

=> fil casreact

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FILE CONTENT:1840 - 17 Nov 2007 VOL 147 ISS 22

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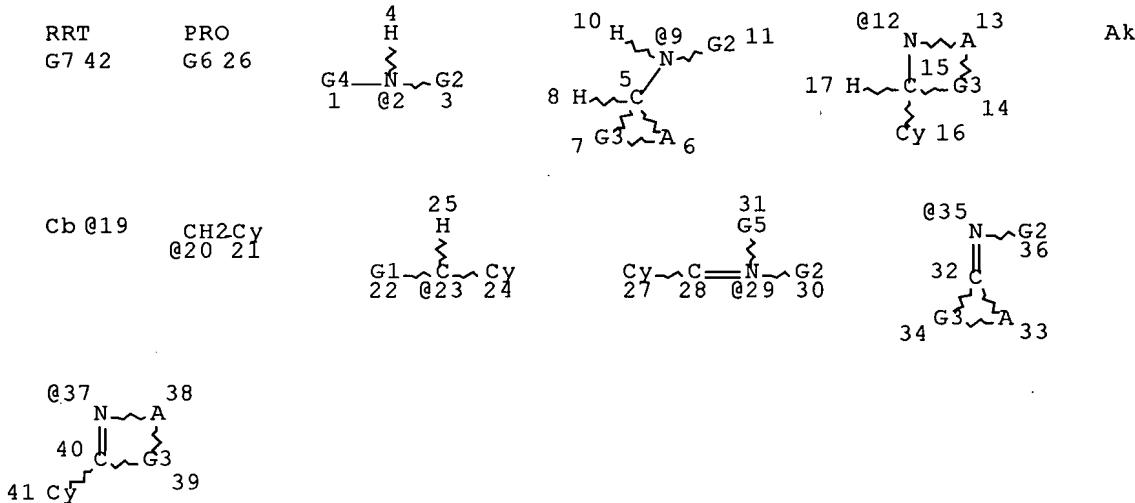
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*

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que 126

L1 STR



Page 1-A

@18

Page 1-B
VAR G1=CY/AK
VAR G2=18/19
REP G3=(0-6) A

VAR G4=20/23

VAR G5=H/CY/AK

VAR G6=2/9/12

VAR G7=29/35/37

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

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GGCAT IS LOC SAT AT 18

GGCAT IS SAT AT 19

GGCAT IS UNS AT 21

GGCAT IS UNS AT 27

GGCAT IS UNS AT 41

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE

L9 STR



NODE ATTRIBUTES:

CONNECT IS E2 RC AT 1

CONNECT IS M2 RC AT 2

CONNECT IS E2 RC AT 3

CONNECT IS M2 RC AT 4

DEFAULT MLEVEL IS ATOM

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GRAPH ATTRIBUTES:

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NUMBER OF NODES IS 5

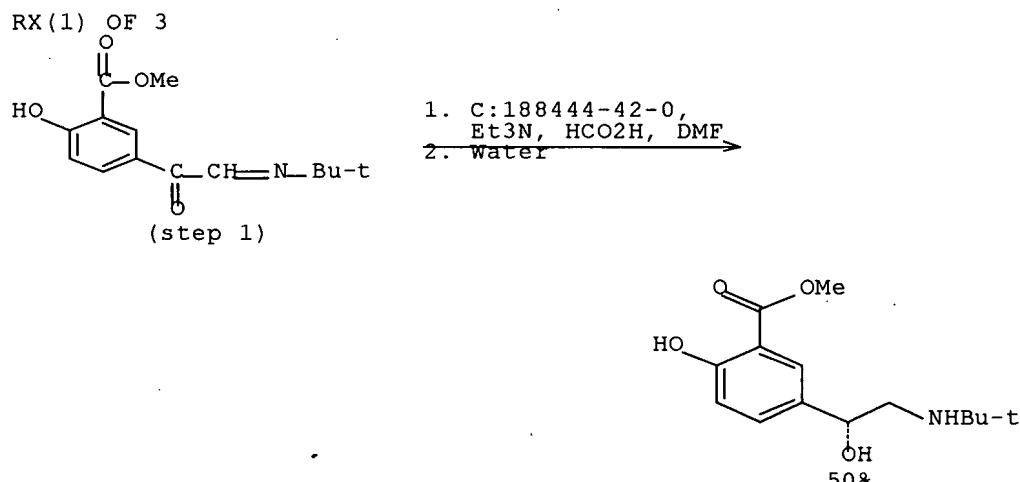
STEREO ATTRIBUTES: NONE

*****MAPPINGS*****

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2	C	RRT	4	C	PRO
3	N	PRO	1	N	RRT
4	C	PRO	2	C	RRT
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L16	1057	SEA FILE=CASREACT SUB=L13	SSS FUL	L1 AND L9 (3799 REACTIONS)	
L17	1057	SEA FILE=CASREACT ABB=ON	PLU=ON	L16/COM	
L18	7887	SEA FILE=CASREACT ABB=ON	PLU=ON	HYDROGENATION/CT	
L19	7167	SEA FILE=CASREACT ABB=ON	PLU=ON	HYDROGENATION CATALYSTS/CT	
L20	91	SEA FILE=CASREACT ABB=ON	PLU=ON	L17 AND L18	
L21	68	SEA FILE=CASREACT ABB=ON	PLU=ON	L20 AND L19	
L26	39	SEA FILE=CASREACT ABB=ON	PLU=ON	L21 AND ?ASYM?	

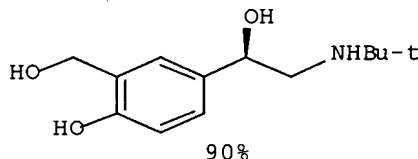
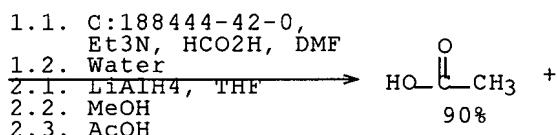
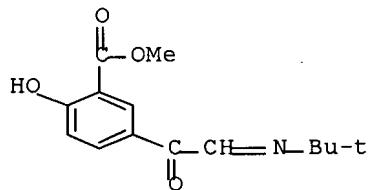
=> d 126 ibib abs crd tot

L26 ANSWER 1 OF 39 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 146:521497 CASREACT Full-text
 TITLE: Synthesis of (R)-salbutamol via asymmetric
 transfer hydrogenation of α -imino-ketone
 AUTHOR(S): Xiao, Yuan-Jing; Yang, Shou-Ning; Shi, Wei; Yang,
 Li-Ping
 CORPORATE SOURCE: Department of Chemistry, East China Normal University,
 Shanghai, 200062, Peop. Rep. China
 SOURCE: Youji Huaxue (2006), 26(8), 1103-1105
 CODEN: YCHHDX; ISSN: 0253-2786
 PUBLISHER: Youji Huaxue Bianjibu
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese
 AB Asym. transfer hydrogenation of α -imino-ketone, i.e., Me 5-[(1,1-dimethylethyl)imino]acetyl]-2-hydroxybenzoate using chiral (S,S)-Ru-TsDPEN [i.e., [N-[(1S,2S)-2-(amino- κ N)-1,2-diphenylethyl]-4-methylbenzenesulfonamido(2-) κ N][(1,2,3,4,5,6- η)-1-methyl-4-(1-methylethyl)benzene]ruthenium] as catalyst, gave the optically pure β -amino-1-arylethanol derivative Me 5-[2-[(1,1-dimethylethyl)amino]-1-hydroxyethyl]-2-hydroxybenzoate, which was reduced to afford (R)-(-)-salbutamol [and (R)-salbutamol acetate].



NOTE: stereoselective, ee 97%, optimization study, optimized on solvent ratio of n(HCOOH):n(Et₃N)
 CON: STAGE {1} room temperature; 24 hours, room temperature
 STAGE {2} room temperature

RX (3) OF 3 - 2 STEPS



NOTE: 1) stereoselective, ee 97%, optimization study, optimized on solvent ratio of n(HCOOH):n(Et₃N)

CON: STEP{1.1} room temperature; 24 hours, room temperature

STEP{1.2} room temperature

STEP{2.1} room temperature; 30 minutes, room temperature;
room temperature -> 45 deg C; 2 hours, 45 deg C

STEP{2.2} 45 deg C

STEP{2.3} room temperature; 10 minutes, room temperature

L26 ANSWER 2 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 146:421415 CASREACT Full-text

TITLE: 1,2-Bis(2,5-diphenylphospholano)methane, a new ligand for asymmetric hydrogenation

AUTHOR(S): Jackson, Mark; Lennon, Ian C.

CORPORATE SOURCE: Dowpharma, Chirotech Technology Ltd., Dow Chemical Company, Cambridge, CB4 0GH, UK

SOURCE: Tetrahedron Letters (2007), 48(10), 1831-1834
CODEN: TELEAY; ISSN: 0040-4039

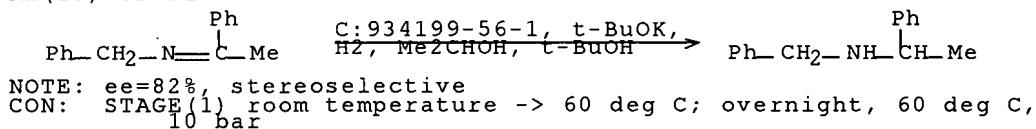
PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 1,2-Bis(2,5-diphenylphospholano)methane (Ph-BPM) was prepared in good yield from 2,5-trans-diphenylphospholane-borane adduct. Rhodium and ruthenium complexes of this ligand were prepared and their usefulness in asym. hydrogenation was investigated. [Ph-BPM Rh(COD)]BF₄ showed high activity and selectivity for itaconate and dehydroamino acid hydrogenation. Ph-BPM RuCl₂(DPEN) was effective for imine hydrogenation.

RX (15) OF 51

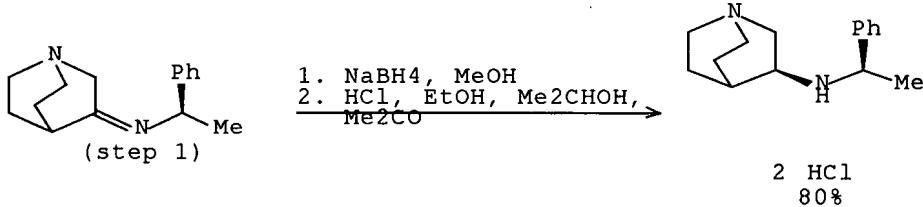


REFERENCE COUNT:

12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 3 OF 39 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 146:100525 CASREACT Full-text
 TITLE: Synthesis of (S)-3-aminoquinuclidine dihydrochloride
 AUTHOR(S): Liu, Yuhai; Wang, Decai
 CORPORATE SOURCE: Pharmaceutical + Life Science College, Nanjing University of Technology, Nanjing, 210009, Peop. Rep. China
 SOURCE: Huagong Shikan (2005), 19(2), 12-13
 CODEN: HUSHFT; ISSN: 1002-154X
 PUBLISHER: Huagong Shikan Zazhishe
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese
 AB (S)-3-Aminoquinuclidine dihydrochloride was synthesized from 3-quinuclidinone HCl and (R)-1-phenethylamine by three steps: ammoniation, reduction with NaBH4, and hydrogenation by 10% Pd/C instead of Pearlman's catalyst. Hydrogenation/deprotection was carried out on (3S)-N-[(1R)-1-phenylethyl]-1-azabicyclo[2.2.2]octan-3-amine dihydrochloride. The total yield was 35%.

RX (3) OF 10



NOTE: stereoselective
 CON: STAGE{1} 0 deg C; 4 hours, cooled
 STAGE{2} pH 1

L26 ANSWER 4 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 145:166887 CASREACT Full-text
 TITLE: Transfer hydrogenation of α -branched ketimines: enantioselective synthesis of cycloalkylamines via dynamic kinetic resolution
 AUTHOR(S): Ros, Abel; Magriz, Antonio; Dietrich, Hansjorg; Ford, Mark; Fernandez, Rosario; Lassaletta, Jose M.
 CORPORATE SOURCE: Instituto de Investigaciones Quimicas (CSIC-USe), Americo Vespuccio s/n, Isla de la Cartuja, Seville, 41092, Spain
 SOURCE: Advanced Synthesis & Catalysis (2005), 347(15),

1917-1920

CODEN: ASCAF7; ISSN: 1615-4150

PUBLISHER:

Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE:

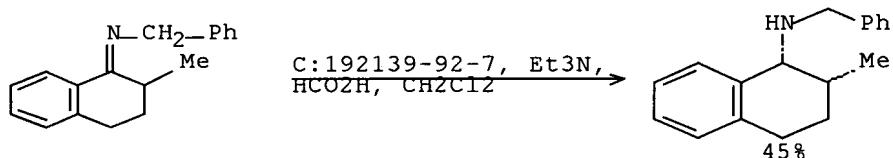
Journal

LANGUAGE:

English

AB The transfer hydrogenation of 2-substituted bicyclic and monocyclic ketimines using $\text{HCO}_2\text{H}/\text{Et}_3\text{N}$ as the hydrogen source and TsDPEN-based Ru(II), Ir(III) and Rh(III) catalysts ((R,R)- and (S,S)- $\text{TsNCHPhCHPhNH}_2\text{RuCl}(\eta^6\text{-p-cymene})$, ((S,S)- $\text{TsNCHPhCHPhNH}_2\text{MCl}(\text{Cp}^*)$ ($\text{M} = \text{Ir, Rh}$)) proceeds with dynamic kinetic resolution to afford the corresponding cis-cycloalkylamines with moderate to excellent levels of diastero- and enantioselectivity. A 1-pot procedure starting from ketones as starting materials with in situ formation of the reacting imines also was developed.

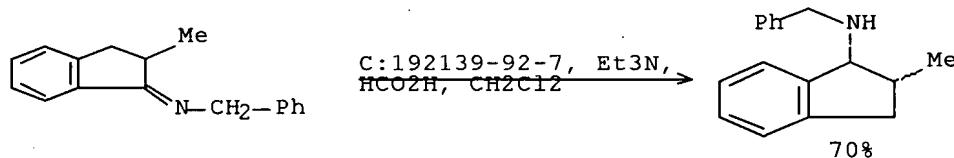
RX(1) OF 18



NOTE: stereoselective, de >98%, ee 50% alternative catalysts ((S,S)- $\text{IrCl}(\text{C}_5\text{Me}_5)\text{TsDPEN}$) or ((S,S)- $\text{RhCl}(\text{C}_5\text{Me}_5)\text{TsDPEN}$) gave near racemic mixture, cis:trans >99:1, dynamic kinetic resolution, Noyori's complex used

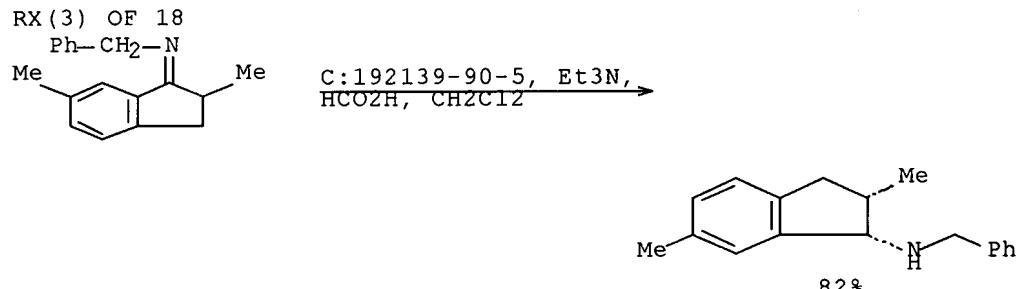
CON: 5 days, room temperature

RX(2) OF 18

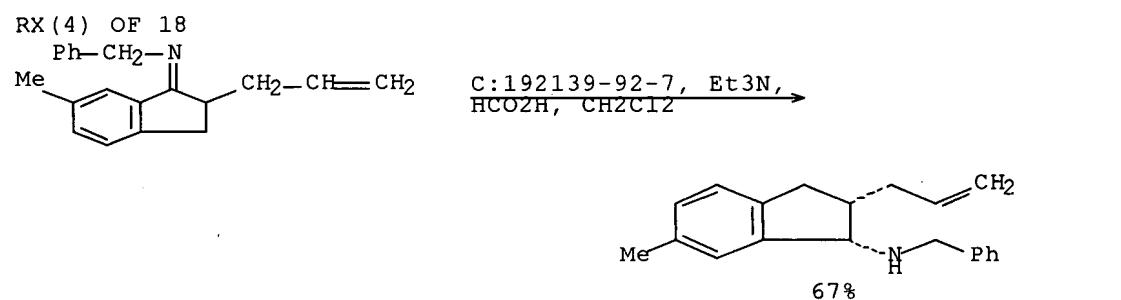


NOTE: stereoselective, de >98%, alternatively catalyst ((S,S)- $\text{IrCl}(\text{C}_5\text{Me}_5)\text{TsDPEN}$) produced other enantiomer in 60% yield with >98% de and 60% ee, ee 96%, cis:trans >99:1, dynamic kinetic resolution, Noyori's complex used

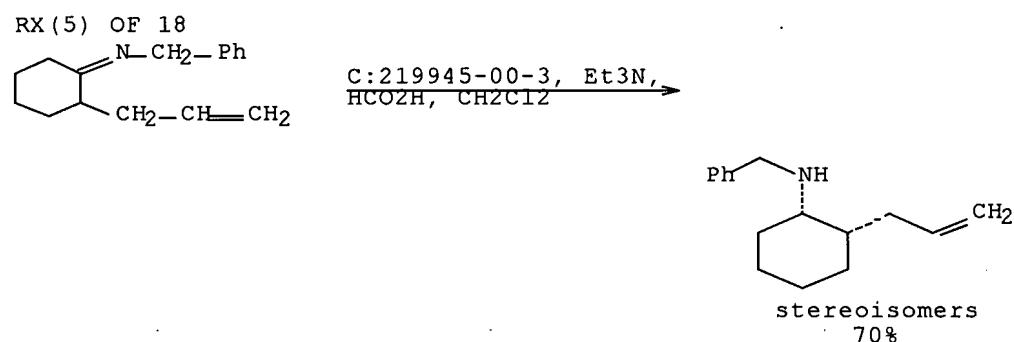
CON: 6 days, room temperature



NOTE: stereoselective, de >98%, ee 97%, cis:trans>99:1, dynamic kinetic resolution
CON: 6 days, room temperature

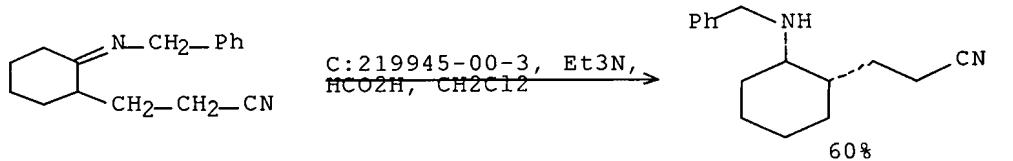


NOTE: stereoselective, de 98%, ee 92%, cis:trans>99:1, dynamic kinetic resolution, alternative catalyst ((S,S)-RuCl(p-cymene)TsDPEN) gave similar yield, Noyori's complex used
CON: 5 days, room temperature



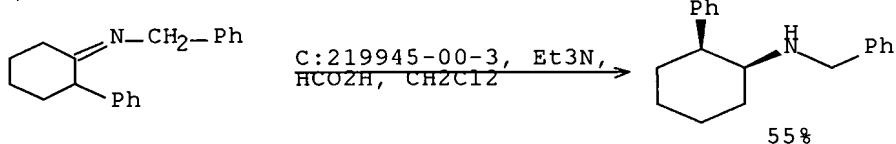
NOTE: stereoselective, de >98%, ee 63%, alternative catalyst ((R,R)-RuCl(p-cymene)TsDPEN) gave racemic isomer, dynamic kinetic resolution
CON: 1 day, room temperature

RX (6) OF 18



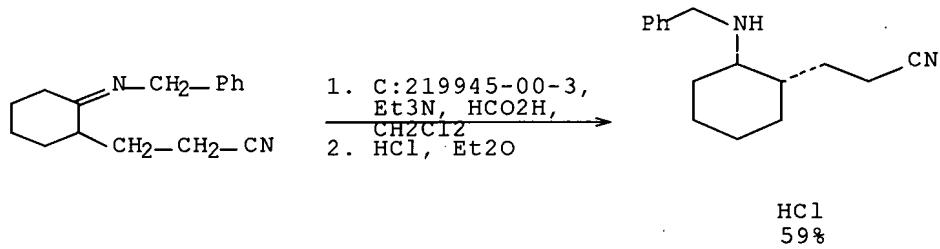
NOTE: stereoselective, de 92%, ee 72%, alternative catalysts ((S,
S)- $\text{RhCl}(\text{C}_5\text{Me}_5)\text{TsDPEN}$) gave low ee and ((R,
R)- $\text{RuCl}(\text{p-cymene})\text{TsDPEN}$) resulted in decomposition,
cis:trans=96:4, dynamic kinetic resolution
CON: 6 days, room temperature

RX (7) OF 18



NOTE: stereoselective, cis:trans>99:1, dynamic kinetic resolution, ee
CON: 50% 1 day, room temperature

RX (16) OF 18 - 2 STEPS



NOTE: 1) stereoselective de 92%, ee 72%, alternative catalysts ((S,
S)- $\text{RhCl}(\text{C}_5\text{Me}_5)\text{TsDPEN}$) gave low ee and ((R,
R)- $\text{RuCl}(\text{p-cymene})\text{TsDPEN}$) resulted in decomposition,
cis:trans=96:4, dynamic kinetic resolution, 2) stereoselective,
de 98% ee 68%, dynamic kinetic resolution
CON: STEP(1) 6 days room temperature
STEP(2) 0 deg C

REFERENCE COUNT:

15

THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 5 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 145:124240 CASREACT Full-text

TITLE: Process for preparing optically active cyclic amines via hydrogenation of imines in presence of chiral catalysts

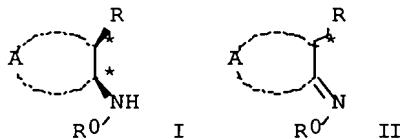
INVENTOR(S): Dietrich, Hansjorg; Ford, Mark James; Muller, Thomas; Lassaletta Simon, Jose Maria; Ros Lao, Abel; Magriz

PATENT ASSIGNEE(S): Tascon, Antonio
 Bayer Cropscience G.m.b.H., Germany
 SOURCE: U.S. Pat. Appl. Publ., 37 pp.
 CODEN: USXXCO

DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

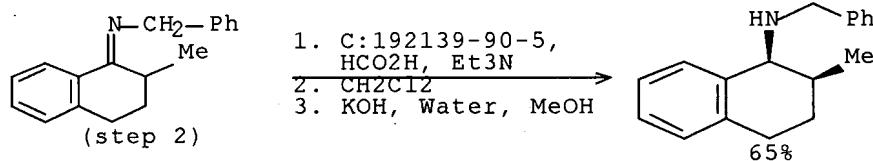
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006149080	A1	20060706	US 2005-320121	20051228
DE 102004063443	A1	20060713	DE 2004-10200406344320041230	
WO 2006072374	A1	20060713	WO 2005-EP13371	20051213
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1833781	A1	20070919	EP 2005-823028	20051213
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
IN 2007CN02940	A	20070907	IN 2007-CN2940	20070702
PRIORITY APPLN. INFO.:			DE 2004-10200406344320041230	
			WO 2005-EP13371	20051213

OTHER SOURCE(S): MARPAT 145:124240
 GI



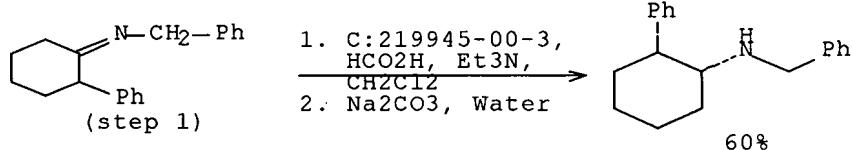
AB Optically active cyclic amines of the formula I [A = (un)saturated, (un)substituted carbocycle or heterocycle; R0 = (un)substituted alkyl, alkenyl, or alkynyl; R = (un)substituted alkyl, alkenyl, alkynyl; R0 and A, or R and A, or R0 and R may also form rings, where R and the NH-R0 group on the two ring carbon atoms marked with an asterisk (*) in each case are arranged in cis arrangement to one another and the stereochemistry on these carbon atoms is different from the racemic configuration], or salts thereof, can be prepared effectively by a process, which comprises converting an imine (a racemic imine) of the formula II via hydrogenation in the presence of hydrogen or a hydrogen donor and a nonenzymic catalyst which comprises a catalytically active optically active complex of one or more transition metals from the group of ruthenium, rhodium, palladium, iridium, osmium, platinum, iron, nickel and samarium with organic ligands, to the compound of the formula I. The process may be carried out on in situ generated imines.

RX(1) OF 3



NOTE: reaction from p. 15 in patent
 CON: STAGE(1) 20 minutes, room temperature
 STAGE(2) 5 days, room temperature
 STAGE(3) room temperature

RX(3) OF 3



NOTE: reaction from p. 16 in patent
 CON: STAGE(1) 24 hours, room temperature
 STAGE(2) room temperature, pH 10

L26 ANSWER 6 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 145:28065 CASREACT Full-text

TITLE: C2-BIPNOR: An Easily Accessible Homologue of BIPNOR for Asymmetric Catalysis

AUTHOR(S): Siutkowski, Magali; Mercier, Francois; Ricard, Louis; Mathey, Francois

CORPORATE SOURCE: Laboratoire Heteroelements et Coordination, Ecole Polytechnique, Palaiseau, 91128, Fr.

SOURCE: Organometallics (2006), 25(10), 2585-2589

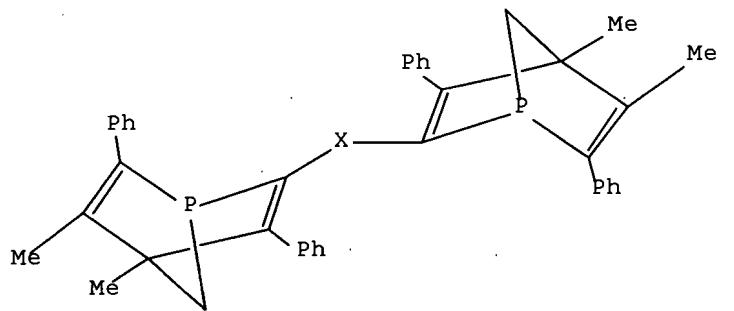
CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

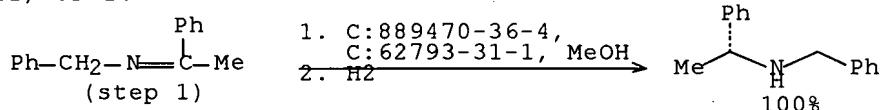
LANGUAGE: English

GI



AB Under mild conditions at -78°, the McMurry coupling of the (R)-2-formyl-1-phosphanorbornadiene 2 yields the enantiopure (RP, SC, SC, RP) diol I (X = CHOHCHOH, 4), dubbed C2-BIPNOR. In boiling THF, the same reaction leads to the trans-alkene I (X = CH:CH 6). C2-BIPNOR is easier to prepare and to handle than BIPNOR while benefiting from the same configurational stability at P. It appears to have a wider range of catalytic applications than BIPNOR and, in one case (asym. Heck reaction), to be competitive with the best ligands proposed in the literature.

RX(11) OF 16



NOTE: stereoselective

CON: STAGE(1) room temperature
STAGE(2) room temperature, 10 atm; 24 hours, 50 deg C

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 7 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:367350 CASREACT Full-text

TITLE: Chiral bis(N-sulfonylamino)phosphine- and TADDOL-phosphite-oxazoline ligands: synthesis and application in asymmetric catalysis

AUTHOR(S): Hilgraf, Robert; Pfaltz, Andreas

CORPORATE SOURCE: Department of Chemistry, University of Basel, Basel, 4056, Switz.

SOURCE: Advanced Synthesis & Catalysis (2005), 347(1), 61-77
CODEN: ASCAF7; ISSN: 1615-4150

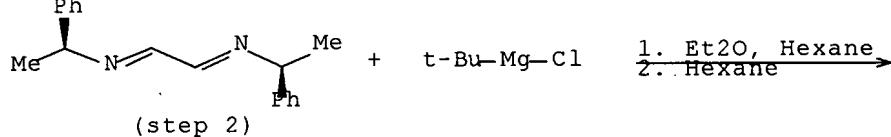
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

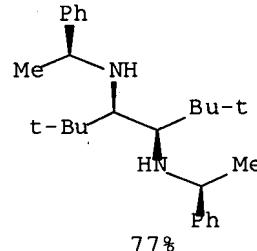
LANGUAGE: English

AB A series of N,P-ligands has been prepared, containing a chiral oxazoline ring and as a second chiral unit a bis(N-sulfonylamino)phosphine group embedded in a diazaphospholidine ring or a cyclic phosphite group derived from TADDOL. These modular ligands are readily synthesized from chiral amino alcs. and chiral 1,2-diamines or TADDOLs. Palladium and iridium complexes derived from these ligands were efficient catalysts for enantioselective allylic alkylation and olefin hydrogenation, resp.

RX (10) OF 102

1. Et₂O, Hexane

2. Hexane



CON: STAGE {1} 20 minutes, 50 deg C
 STAGE {2} 45 minutes, 50 deg C

REFERENCE COUNT:

28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 8 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:248056 CASREACT Full-text

TITLE: Enantioselective hydrogenation of alkenes and imines by a gold catalyst

AUTHOR(S): Gonzalez-Arellano, Camino; Corma, Avelino; Iglesias, Marta; Sanchez, Felix

CORPORATE SOURCE: Instituto de Quimica Organica General, CSIC, Madrid, 28006, Spain

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2005), (27), 3451-3453

CODEN: CHCOFS; ISSN: 1359-7345

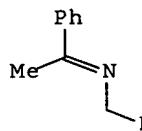
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

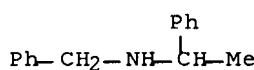
AB A new neutral dimeric gold(I) complex bearing the 1,2-bis[(2R,5R)-2,5-dimethylphospholanebenzene] [(R,R)-Me-Duphos] ligand has been synthesized which catalyzes the asym. hydrogenation of alkenes and imines under mild reaction conditions.

RX (5) OF 13

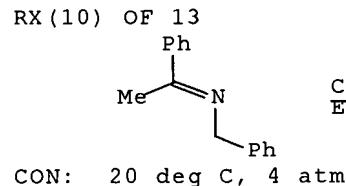
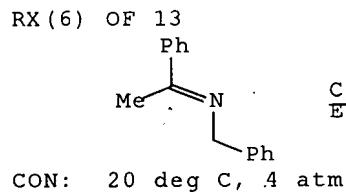


C:863238-51-1, H2,

EtOH



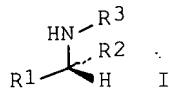
CON: 20 deg C, 4 atm



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

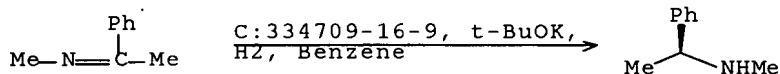
L26 ANSWER 9 OF 39 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 143:78085 CASREACT Full-text
 TITLE: A preparation of amines via asymmetric ruthenium-catalyzed hydrogenation of imines
 INVENTOR(S): Abdur-Rashid, Kamaluddin
 PATENT ASSIGNEE(S): Can.
 SOURCE: PCT Int. Appl., 50 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005056513	A1	20050623	WO 2004-CA2130	20041215
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2549929	A1	20050623	CA 2004-2549929	20041215
PRIORITY APPLN. INFO.:			US 2003-529084P	20031215
			WO 2004-CA2130	20041215
OTHER SOURCE(S): GI		MARPAT 143:78085		



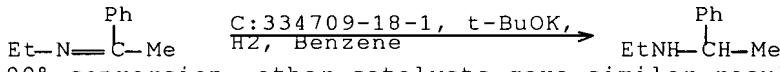
AB The invention relates to a preparation of amines of formula I [wherein: R1 is (hetero)aryl; R2 is H, (hetero)aryl, alkyl, or alk(en/yn)yl, etc.; and R3 is (cyclo)alkyl] via ruthenium-catalyzed hydrogenation of imines of formula R1(R2)C=NR3. The catalytic system includes a ruthenium complex containing (1) a diamine and (2) a diphosphine or two monodentate phosphines ligands. Such process also relates to the asym. hydrogenation of prochiral imines to the chiral amines using chiral ruthenium complexes bearing chiral diphosphines or chiral monodentate phosphines and chiral diamines. For instance, (S)-Ph(Me)CHNH(Me) was prepared via asym. Ru-catalyzed hydrogenation of N-(1-phenylethylidene)methylamine (conversion: 97%, ee: 71%).

RX (2) OF 15



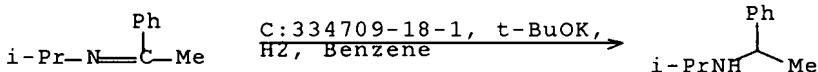
NOTE: optimization study (optimized on catalyst), stereoselective
CON: 24 hours, room temperature, 30 bar

RX (5) OF 15



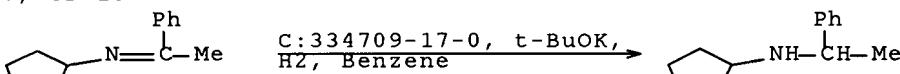
NOTE: 100% conversion, other catalysts gave similar results
CON: 24 hours, room temperature, 30 bar

RX (6) OF 15



NOTE: 91% conversion, other catalysts gave similar results
CON: 24 hours, room temperature, 50 bar

RX (7) OF 15

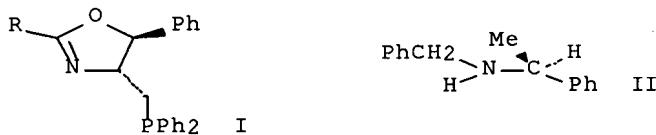


NOTE: 97% conversion, other catalysts gave similar results
CON: 24 hours, room temperature, 50 bar

REFERENCE COUNT:

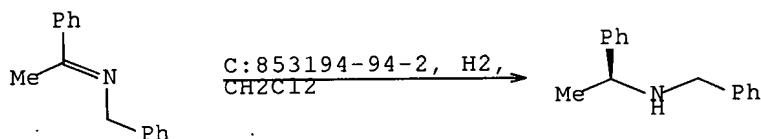
3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 10 OF 39 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 143:43922 CASREACT Full-text
 TITLE: New chiral N,P-oxazolines, and their Ir complexes in asymmetric hydrogenation of an imine
 AUTHOR(S): Ezhova, Maria B.; Patrick, Brian O.; James, Brian R.; Waller, Francis J.; Ford, Michael E.
 CORPORATE SOURCE: Department of Chemistry, The University of British Columbia, Vancouver, BC, V6T 1Z1, Can.
 SOURCE: Journal of Molecular Catalysis A: Chemical (2004), 224(1-2), 71-79
 CODEN: JMCCF2; ISSN: 1381-1169
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



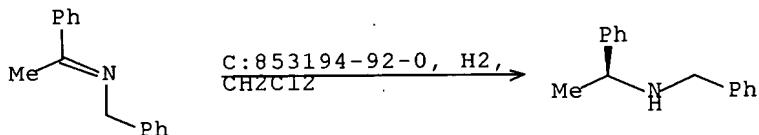
AB (+) (1S,2S)-2-Amino-1-phenyl-1,3-propanediol reacts with ortho-esters to form 4-hydroxymethyl-5-phenyl-1,3-oxazolines. Subsequent reaction of their toluenesulfonyl derivs. with diphenylphosphinolithium yields the N,P-ligands, (4S,5S)-2-R-4-diphenylphosphinomethyl-5-phenyl-1,3-oxazoline I (R = Me, Et, Ph). X-ray analyses of (4S,5S)-2-methyl-4-toluenesulfonylmethyl-5-phenyl-1,3-oxazoline and (4S,5S)-2,5-diphenyl-4-diphenylphosphinomethyl-1,3-oxazoline reveal retention of absolute configuration throughout the synthesis. The [Ir(COD)(N,P-oxazoline)]PF₆ systems in CH₂Cl₂ effect catalytic hydrogenation of N-(1-phenylethylidene)benzylamine, PhCH₂N = C(Me)Ph, to the corresponding amine II with up to 63% e.e. with the R = Et ligand.

RX(13) OF 35



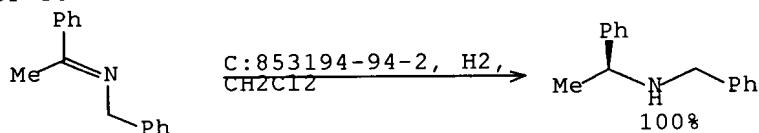
NOTE: stereoselective, yield depends on amount of catalyst, yield depends on amount of catalyst, temperature, pressure, yield depends on amount of catalyst, temperature, pressure, solvent
CON: 3 hours, 80 deg C, 55 atm

RX(14) OF 35



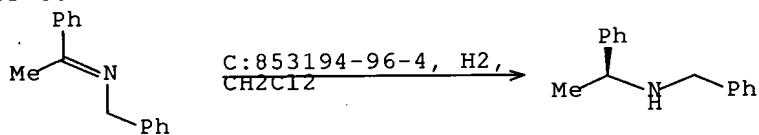
NOTE: stereoselective, yield depends on amount of catalyst, yield depends on amount of catalyst, temperature, pressure, yield depends on amount of catalyst, temperature, pressure, solvent
CON: 5 hours, 80 deg C, 55 atm

RX(16) OF 35



NOTE: stereoselective, yield depends on amount of catalyst, yield depends on amount of catalyst, temperature, pressure, yield depends on amount of catalyst, temperature, pressure, solvent
CON: 2 hours, 22 deg C, 3 atm

RX(17) OF 35



NOTE: stereoselective, yield depends on amount of catalyst, temperature, pressure, solvent
CON: 5 hours, 80 deg C, 55 atm

REFERENCE COUNT:

66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 11 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 142:93172 CASREACT Full-text

TITLE: An efficient method for the synthesis of enantiopure phosphine-imidazoline ligands: application to the Ir-catalyzed hydrogenation of imines

AUTHOR(S): Guiu, Ester; Claver, Carmen; Benet-Buchholz, Jordi;

CORPORATE SOURCE:

Castillon, Sergio

SOURCE:

Departament de Quimica Analitica i Quimica Organica,
Universitat Rovira i Virgili, Tarragona, 43005, Spain
Tetrahedron: Asymmetry (2004), 15(21), 3365-3373
CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER:

Elsevier B.V.

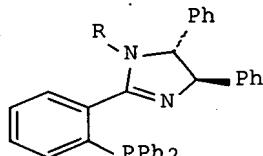
DOCUMENT TYPE:

Journal

LANGUAGE:

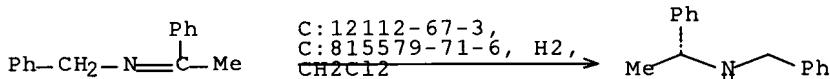
English

GI



AB Phosphine-imidazoline ligands I ($R = H, F3CCO, PhCH_2$) were synthesized from 2-(2-haloaryl)imidazolines, which have previously been obtained from dithioesters. The coordination of ligand I ($R = H$) to Ir(I) was studied and the mol. structure of the complex of I ($R = H$) with $[Ir(\eta^4\text{-COD})]BF_4$ (COD = 1,5-cyclooctadiene) determined by X-ray diffraction. The in situ prepared Ir(I)/phosphine-imidazoline catalysts were tested in the asym. hydrogenation of ketimines in order to evaluate the influence of the electronic parameters of the ligand on the catalytic reaction.

RX (9) OF 29



NOTE: high pressure, 44% conversion, other catalysts gave higher conversion but poorer stereoselectivity
CON: 16 hours, room temperature, 70 bar

REFERENCE COUNT:

66

THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 12 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 142:55874 CASREACT Full-text

TITLE: Process for producing optically active

1-alkyl-substituted 2,2,2-trifluoroethylamine

INVENTOR(S): Ishii, Akihiro; Kuriyama, Yokusu; Yasumoto, Manabu;
Kanai, Masatomi; Inomiya, Kenjin; Ootsuka, Takashi;
Ueda, Koji

PATENT ASSIGNEE(S): Central Glass Company, Limited, Japan

SOURCE: PCT Int. Appl., 31 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

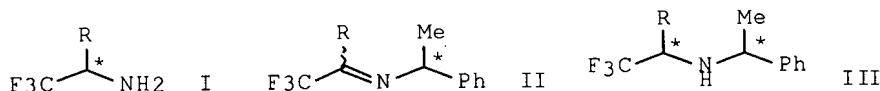
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004110977	A1	20041223	WO 2004-JP7955	20040608
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2005002036	A	20050106	JP 2003-166525	20030611
EP 1642884	A1	20060405	EP 2004-745665	20040608
R: DE, FR, GB				
CN 1832918	A	20060913	CN 2004-80022700	20040608
US 2006281950	A1	20061214	US 2006-560251	20060516
PRIORITY APPLN. INFO.:			JP 2003-166525	20030611
			WO 2004-JP7955	20040608

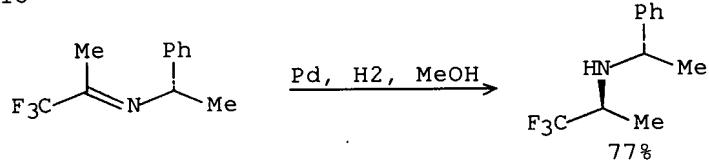
OTHER SOURCE(S): MARPAT 142:55874
GI



AB There is provided a process for producing an optically active, 1-alkyl-substituted 2,2,2-trifluoroethylamine represented by the formula (I) (wherein R represents C1-6 alkyl and * indicates asym. carbon) or a salt of the compound. The process comprises asym. reducing an optically active imine represented by the formula (E)- or (Z)-(II) (R, * = same as above) with the aid of a catalyst comprising a Group VIII metal in a hydrogen atmospheric to convert it to an optically active secondary amine represented by the formula (III) (R, * = same as above) and subjecting the secondary amine or a salt thereof to hydrogenolysis to produce the target compound. These compds. are important intermediates for medicines and agricultural chems. Thus, a solution of 734.38 g (S)-1-phenylethylamine in 1,000 mL toluene was added to a solution of 1,158.56 g 1,1,1-trifluoroacetone in 4,600 mL toluene under ice-cooling, stirred at 32-34° for 2 h, and the reaction mixture was treated with 57.64 g pyridinium p-toluenesulfonate monohydrate and stirred at 60-84° for 7 h 30 min to give, after workup and distillation at 1,200-1,330 Pa and 79-85°, 73% N-(E)-(2,2,2-trifluoroisopropylidene)-(S)-1-phenylethylamine (IV). IV (10.411 kg) and 0.521 kg 5% Pd-C (50 weight% wet) were added to 48.382 L MeOH, cooled to 0°, and hydrogenated at 0.50-0.52 MPa, -1° to 0° for 53 h 40 min to give, after filtration through celite, evaporation of the solvent, and distillation, 77% N-(2,2,2-trifluoroisopropyl)-(S)-1-phenylethylamine (V) in a S-S:R-S isomer ratio of 70:30. V was converted into the HBr salt by treating the filtrate of the above step with 48% aqueous HBr and the HBr salt was recrystd. from isopropanol to give N-((S)-2,2,2-trifluoroisopropyl)-[(S)-1-phenylethyl]amine hydrobromide (94.9% d.e.) which was treated with 1 N aqueous NaOH and extracted with EtOAc to give N-((S)-2,2,2-

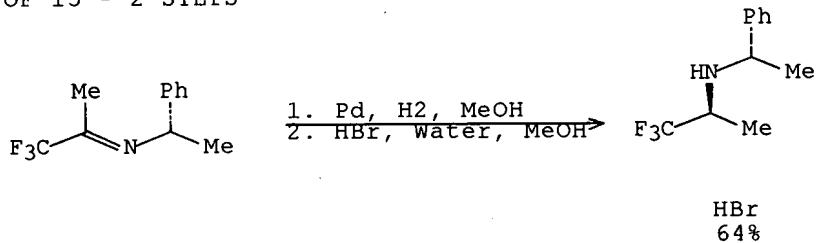
trifluoroisopropyl)-[(S)-1-phenylethyl]amine (VI). VI (6.60 g) was hydrogenolyzed over 0.33 g 5% Pd-C in 30 mL MeOH at 0.5-0.6 MPa and 60-62° for 15 h to give, after filtration through celite, adding 10% methanolic HCl to the filtrate, and concentration under reduced pressure, 90% crude (S)-1-methyl-2,2,2-trifluoroethylamine hydrochloride.

RX (2) OF 15



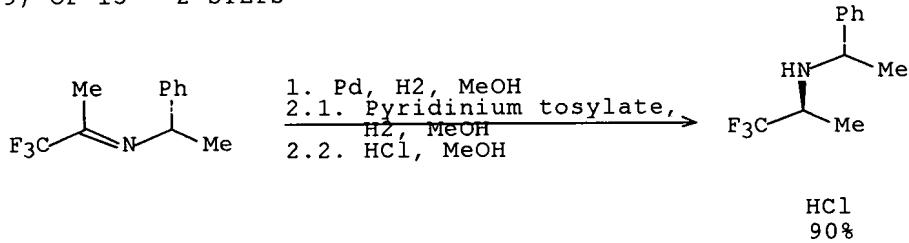
NOTE: stereoselective hydrogenation over 5% Pd/C
CON: 53.7 hours, -1 deg C → 0 deg C, 0.50e+6 Pa → 0.52e+6 Pa

RX (8) OF 15 - 2 STEPS



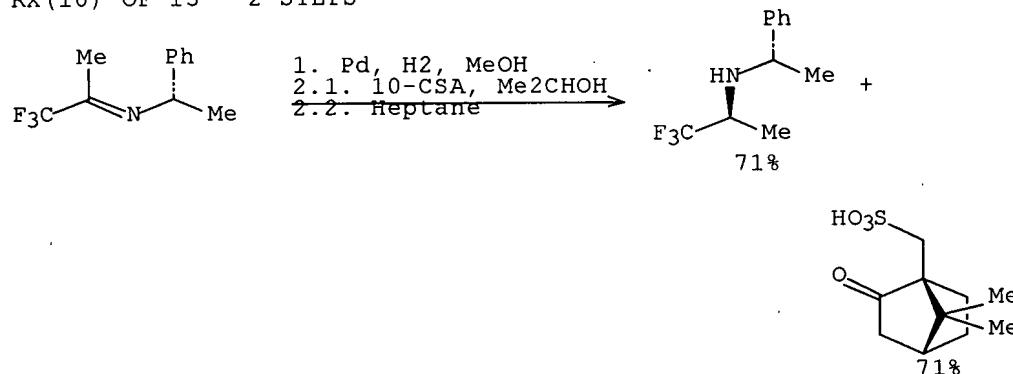
NOTE: 1) stereoselective hydrogenation over 5% Pd/C, 2) salt formation;
two crystns from isopropanol
CON: STEP(1) 53.7 hours, -1 deg C → 0 deg C,
0.50e+6 Pa → 0.52e+6 Pa
STEP(2) room temperature

RX (9) OF 15 - 2 STEPS



NOTE: 1) stereoselective hydrogenation over 5% Pd/C, 2) hydrogenolysis
over 5% Pd/C; salt formation
CON: STEP(1) 53.7 hours, -1 deg C → 0 deg C,
0.50e+6 Pa → 0.52e+6 Pa
STEP(2.1) 15 hours, 6062 deg C, 5e+5 Pa → 6e+5 Pa
STEP(2.2) room temperature

RX(10) OF 15 - 2 STEPS



NOTE: 1) stereoselective hydrogenation over 5% Pd/C, 2) crystn. and purifn.
 CON: STEP{1} 53.7 hours -1 deg C -> 0 deg C,
 $0.50e+6$ Pa -> $0.52e+6$ Pa
 STEP{2.1} 80 deg C
 STEP{2.2} 80 deg C -> 25 deg C; overnight, 25 deg C

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 13 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 141:410655 CASREACT Full-text

TITLE: Application of Phosphine-Oxazoline Ligands in Ir-Catalyzed Asymmetric Hydrogenation of Acyclic Aromatic N-Arylimines

AUTHOR(S): Trifonova, Anna; Diesen, Jarle S.; Chapman, Christopher J.; Andersson, Pher G.

CORPORATE SOURCE: Department of Chemistry Organic Chemistry, Uppsala University, Uppsala, SE-75124, Swed.

SOURCE: Organic Letters (2004), 6(21), 3825-3827
CODEN: ORLEF7; ISSN: 1523-7060

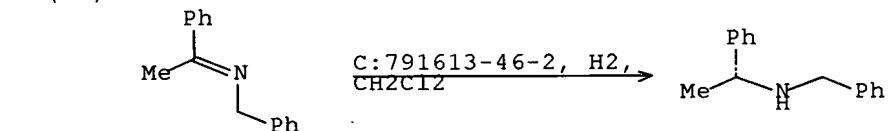
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new class of chiral phosphine-oxazoline ligands have been developed. Chiral Ir complexes prepared from these ligands induced high enantioselectivities (66-90% ee) when applied to the asym. hydrogenation of acyclic aromatic N-arylimines, e.g. PhCMe:NPh.

RX(18) OF 32



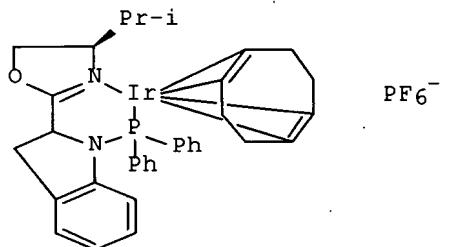
NOTE: high pressure, stereoselective, 63% conversion, 66% ee
 CON: 12 hours, room temperature, 20 bar

REFERENCE COUNT:

54

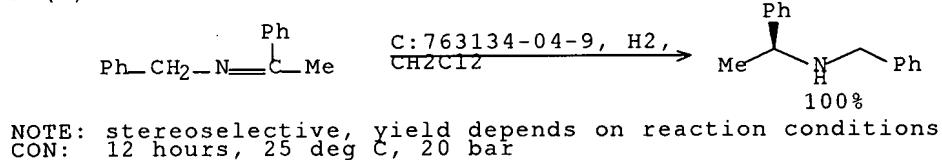
THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 14 OF 39 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 141:295668 CASREACT Full-text
 TITLE: Efficient enantioselective hydrogenation of arylimines using aminophosphine-oxazoline iridium catalysts
 AUTHOR(S): Blanc, Catherine; Agbossou-Niedercorn, Francine; Nowogrocki, Guy
 CORPORATE SOURCE: UMR CNRS 8010, ENSCL, Laboratoire de Catalyse de Lille, Villeneuve d'Ascq, 59652, Fr.
 SOURCE: Tetrahedron: Asymmetry (2004), 15(14), 2159-2163
 CODEN: TASYE3; ISSN: 0957-4166
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The preparation and characterization of cationic iridium complexes bearing chiral aminophosphine-oxazoline auxiliaries of general formula $[Ir(COD)L^*]X$ [$X: PF_6^-$ and $B(ArF)_4^-$] is reported. These complexes have been applied to the asym. hydrogenation of two imines: N-(phenylethyldene)aniline and N-(phenylethyldene)benzylamine providing the corresponding chiral amines in up to 90% and 82% ee, resp. The reaction of di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]diiridium with (2S)-2-[(4R)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl]-1-(diphenylphosphino)-2,3-dihydro-1H-indole gave a chiral [2-[(4R)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl]-1-(diphenylphosphino)-2,3-dihydro-1H-indole]-iridium complex (I). The stereoselective hydrogenation of N-(1-phenylethyldene)benzenamine using I as catalyst gave (α S)- α -methyl-N-phenylbenzenemethanamine. The effect of changing the counter ion was briefly examined. The catalytic activity of (3S)-3-[(4R)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl]-2-(diphenylphosphino)-1,2,3,4-tetrahydroisoquinoline-iridium complex was compared to a chiral PHOX-iridium complex (chiral auxiliary) and found to be comparable in catalytic activity. The crystal and mol. structures of I-tetrakis[3,5-bis(trifluoromethyl)phenyl]borate were reported.

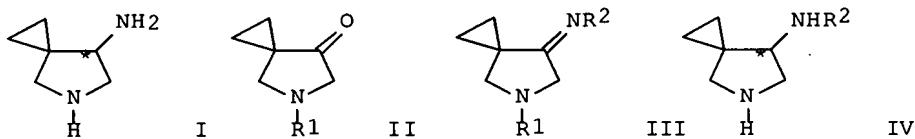
RX (8) OF 9



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 15 OF 39 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 140:303521 CASREACT Full-text
 TITLE: Method for preparation of optically active 7-amino-5-azaspiro[2.4]heptane
 INVENTOR(S): Muto, Makoto; Nakayama, Takashi; Akiba, Toshifumi;
 Saga, Tetsuya
 PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan; Daiichi Fine Chemical Co., Ltd.
 SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

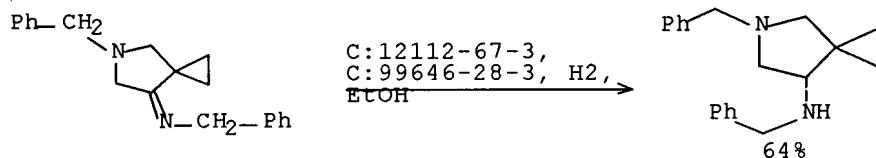
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004099609	A	20040402	JP 2003-298180	20030822
PRIORITY APPLN. INFO.:	JP 2002-243510 20020823			
OTHER SOURCE(S):	MARPAT 140:303521			
GI				



AB Optically active 7-amino-5-azaspiro[2.4]heptane (I; * denotes an asym. carbon atom) is prepared by reaction of 5-azaspiro[2.4]heptan-7-one (II; R1 = H, amino-protecting group) with an amine of formula R2-NH2 (R2 = H, amino-protecting group), and reduction of the resulting 7-imino-5-azaspiro[2.4]heptane (III; R1, R2 = same as above) in the presence of an asym. catalyst represented by formula MXaLn (M = group 8 to 10 transition metal in the periodic table; X = H, halo, alkoxy, alkenyl, aryl; L = an optically active phosphine ligand; m = an integer of 0-6) or reduction of optically active III [R2 = an amino or imino protecting group having an asym. carbon atom, e.g. (R)-1-phenylethyl], and optional deprotection of the resulting optically active amine (IV; R1, R2 = same as above). Thus, 0.1 mL Et2O.BF3 was added to a solution of 1 g 5-benzyl-5-azaspiro[2.4]heptan-7-one and 642 mg

benzylamine in 10 mL benzene and refluxed for 4 h with removing water through a Dean-Stark trap, followed by distillation of the solvent and purification using silica gel chromatog., to give 952 mg N-benzyl-N-(5-benzyl-5-azaspiro[2.4]hept-7-ylidene)amine (V). (R)-tol-BINAP (67.9 mg) was added to a solution of 30.9 mg [Ir(COD)Cl]₂ (30.9 mg) in 4.5 mL ethanol, stirred at room temperature for 2 h to prepare a catalyst solution. A solution of 290 mg V in 4.5 mL ethanol and the latter catalyst solution were added to an autoclave and stirred at -10° for 63 h under 30 atm H pressure to give, distillation of the solvent under reduced pressure and silica gel chromatog., 187 mg (7S)-N-benzyl-N-(5-benzyl-5-azaspiro[2.4]heptan-7-yl)amine (VI) (64%, 53% e.e.). VI (170 mg) and 17 mg 5% Pd-C was suspended in 2 mL toluene, treated with 0.58 mL concentrated HCl, stirred under H atmospheric for 5 h, filtered, treated with 5 mL iso-Pr alc., stirred for 3 h, and filtered to give 177 mg (7S)-7-amino-5-azaspiro[2.4]heptane dihydrochloride.

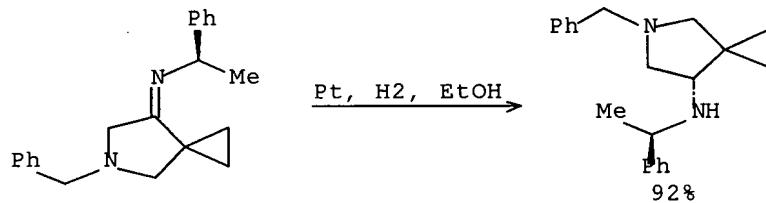
RX(2) OF 13



NOTE: catalyst prepn. and high pressure stereoselective (asym.) hydrogenation; 53% e.e.

CON: STAGE(1) 2 hours, room temperature; 63 hours, -10 deg C, 30 atm

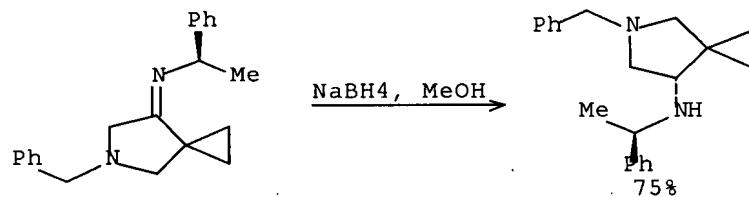
RX(5) OF 13



NOTE: stereoselective hydrogenation; 7S/7R isomer ratio of 97/3

CON: 44 hours, 45 deg C

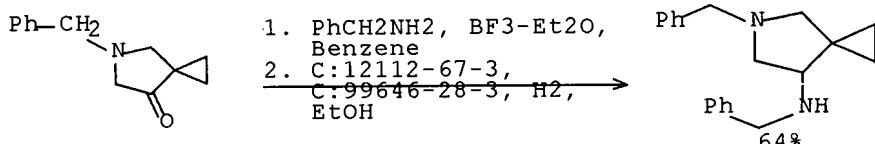
RX(6) OF 13



NOTE: stereoselective redn.; 7S/7R isomer ratio of 94/6

CON: 2 hours, room temperature

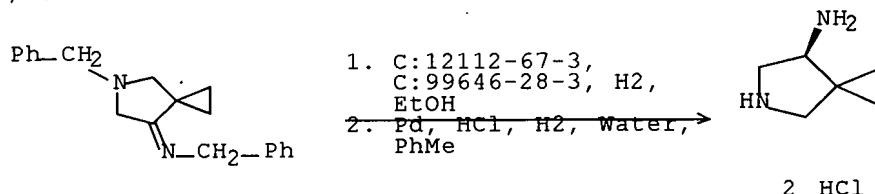
RX(8) OF 13 - 2 STEPS



NOTE: 1) imination with removal of water, 2) catalyst prepn. and high pressure stereoselective (asym.) hydrogenation; 53% e.e.

CON: STEP{1} 4 hours, reflux
STEP{2.1} 2 hours, room temperature; 63 hours, -10 deg C, 30 atm

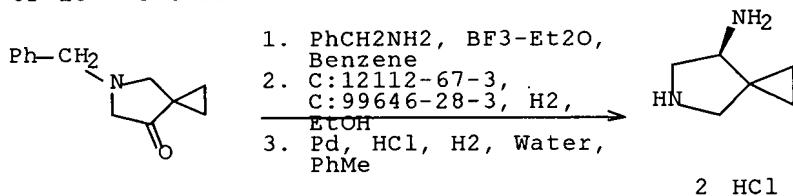
RX(9) OF 13 - 2 STEPS



NOTE: 1) catalyst prepn. and high pressure stereoselective (asym.) hydrogenation; 53% e.e., 2) hydrogenolysis (debenzylation)

CON: STEP{1.1} 2 hours, room temperature; 63 hours, -10 deg C, 30 atm
STEP{2} 5 hours, room temperature

RX(12) OF 13 - 3 STEPS



NOTE: 1) imination with removal of water, 2) catalyst prepn. and high pressure stereoselective (asym.) hydrogenation; 53% e.e., 3) hydrogenolysis (debenzylation)

CON: STEP{1} 4 hours, reflux
STEP{2.1} 2 hours, room temperature; 63 hours, -10 deg C, 30 atm
STEP{3} 5 hours, room temperature

L26 ANSWER 16 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 140:235900 CASREACT Full-text

TITLE:

Preparation of chiral diphosphines and their transition metal complexes and their use in asymmetric synthesis

INVENTOR(S):

Meseguer, Benjamin; Militzer, Hans-Christian;
Castillon, Sergio; Claver, Carmen; Diaz, Yolanda;
Aghmiz, Mohamed; Guiu, Esther; Aghmiz, Ali; Masdeu,
Anna

PATENT ASSIGNEE(S):

Bayer A.-G., Germany

SOURCE: Ger. Offen., 34 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

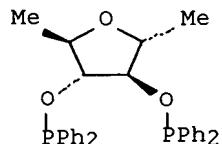
FAMILY ACC.. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10241256	A1	20040304	DE 2002-10241256	20020906
EP 1400527	A1	20040324	EP 2003-18221	20030811
EP 1400527	B1	20060322		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
AT 321059	T	20060415	AT 2003-18221	20030811
ES 2259400	T3	20061001	ES 2003-3018221	20030811
IN 2003DN00996	A	20050527	IN 2003-DN996	20030814
US 2005080047	A1	20050414	US 2003-643552	20030819
US 7193092	B2	20070320		
JP 2004161741	A	20040610	JP 2003-208112	20030820
CN 1493576	A	20040505	CN 2003-158087	20030821
US 2007155971	A1	20070705	US 2007-707710	20070216
PRIORITY APPLN. INFO.:			DE 2002-10238115	20020821
			DE 2002-10241256	20020906
			US 2003-643552	20030819

OTHER SOURCE(S): MARPAT 140:235900

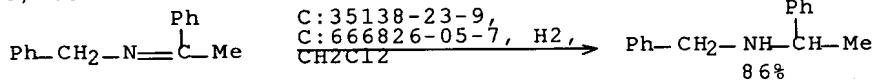
GI



I

AB The present invention concerns the preparation of chiral diphosphines their transition metal complexes, and use of complexes in asym. syntheses. Thus, preparation of 2,3-bis-O-(diphenylphosphino)-1,6-dideoxy-2,5-anhydro-D-mannitol I, prepared from 1,6-dideoxy-2,5-anhydro-D-mannitol, and [Rh(cod)₂]BF₄/I catalyzed enantioselective hydrogenation of CH₂:C(NHAc)(CO₂Me) is described.

RX (35) OF 78



NOTE: stereoselective
 CON: 16 hours, 25 deg C, 70 atm

L26 . ANSWER 17 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 140:93769 CASREACT Full-textTITLE: (S)-1-Aminoindane: synthesis by chirality transfer
using (R)-phenylglycine amide as chiral auxiliaryAUTHOR(S): Uiterweerd, Patrick G. H.; van der Sluis, Marcel;
Kaptein, Bernard; de Lange, Ben; Kellogg, Richard M.;
Broxterman, Quirinus B.

CORPORATE SOURCE: Syncom B.V., Groningen, 9747 AT, Neth.

SOURCE: Tetrahedron: Asymmetry (2003), 14(22), 3479-3485

CODEN: TASYE3; ISSN: 0957-4166

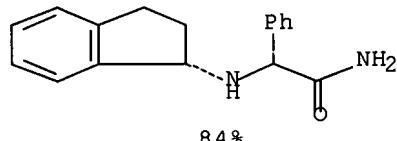
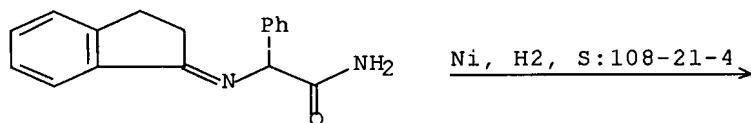
PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A practical asym. synthesis of nearly enantiomerically pure (S)-1-aminoindane has been developed. The key step involves the diastereoselective heterogeneous metal-catalyzed reduction of the ketimine of 1-indanone with the chiral auxiliary (R)-phenylglycine amide. The reduction of (α R)- α -[(2,3-dihydro-1H-inden-1-ylidene)amino]benzeneacetamide gave (α R)- α -[(1S)-2,3-dihydro-1H-inden-1-yl]amino]benzeneacetamide. The latter was converted to (α R)- α -[(1S)-2,3-dihydro-1H-inden-1-yl]amino]benzeneacetonitrile and then into (1S)-2,3-dihydro-N-(phenylmethylene)-1H-inden-1-amine, which is a precursor for (+)-(1S)-2,3-Dihydro-1H-inden-1-amine. The selectivity of the asym. hydrogenation step was optimized with regard to metal catalyst, solvent and catalyst loading. The chiral auxiliary was removed by means of a novel non-reductive procedure. Thus, (S)-1-aminoindane with an ee of 96% was prepared in 58% overall yield from (R)-phenylglycine amide in an effective three-step procedure.

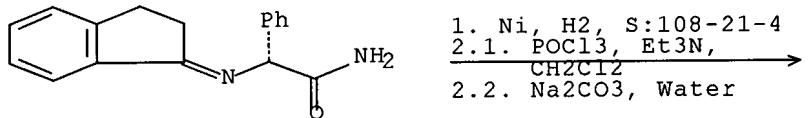
RX (2) OF 16



84%

NOTE: stereoselective, Raney nickel used, optimization study,
optimized on catalyst, solvent, temperature and timeCON: STAGE(1) room temperature, 3.5 atm; room temperature -> 40 deg C;
45 hours, 40 deg C

RX (8) OF 16 - 2 STEPS



NOTE: 1) stereoselective, Raney nickel used, optimization study, optimized on catalyst, solvent, temperature and time

CON: STEP(1.1) room temperature, 3.5 atm;
room temperature -> 40 deg C; 45 hours, 40 deg C
STEP(2.1) room temperature; room temperature -> 0 deg C; 0 deg C;
10 minutes, 0 deg C; 0 deg C -> room temperature; 60 minutes,
room temperature
STEP(2.2) pH 8

REFERENCE COUNT:

26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 18 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 139:52706 CASREACT Full-text

TITLE: Iridium-catalyzed enantioselective hydrogenation of imines with xylose diphosphite and diphosphinite ligands

AUTHOR(S): Guiu, Ester; Munoz, Bianca; Castillon, Sergio; Claver, Carmen

CORPORATE SOURCE: Departament de Quimica Fisica i Inorganica and Departament de Quimica Analitica i Quimica Organica, Universitat Rovira i Virgili, Pl. Imperial Tarraco 1, Tarragona, 43005, Spain

SOURCE: Advanced Synthesis & Catalysis (2003), 345(1+2), 169-171

CODEN: ASCAF7; ISSN: 1615-4150

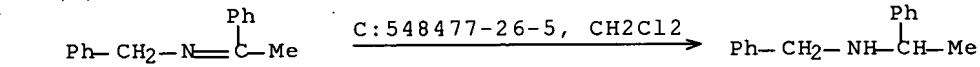
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

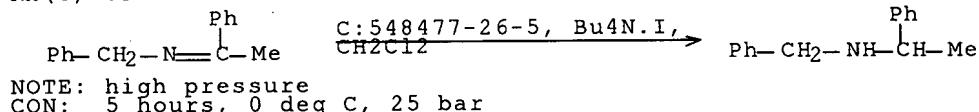
AB Iridium complexes incorporating xylose diphosphinite phosphite ligands as source of chirality are active catalysts for the hydrogenation of imines providing moderate ee. The enantioselectivity depends on the fine tuning of the structural parameters of the ligand and on the effect of additives.

RX (4) OF 6



NOTE: high pressure
CON: 16 hours, 25 deg C, 50 bar

RX(6) OF 6



REFERENCE COUNT:

28

THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 19 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 139:52705 CASREACT Full-text

TITLE: Synthesis of chiral trifluoromethylated amines by palladium-catalyzed diastereoselective hydrogenation-hydrogenolysis approach

AUTHOR(S): Torok, Bela; Prakash, G. K. Surya

CORPORATE SOURCE: Donald P. and Katherine B. Loker Hydrocarbon Research Institute and Department of Chemistry, University of Southern California, Los Angeles, CA, 90089-1661, USA

SOURCE: Advanced Synthesis & Catalysis (2003), 345(1+2), 165-168

CODEN: ASCAF7; ISSN: 1615-4150

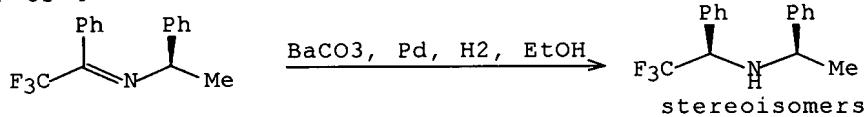
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

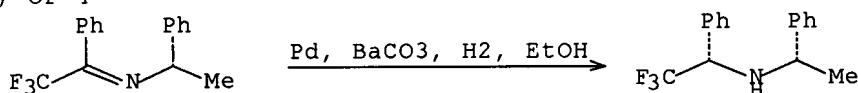
AB The synthesis of chiral 2,2,2-trifluoro-1-phenylethylamines by palladium-catalyzed diastereoselective heterogeneous catalytic hydrogenation is described. The one-pot process involves two steps; the diastereoselective hydrogenation of chiral 2,2,2-trifluoro-1-phenylethyl-N-1'-phenylethylimines and the hydrogenolysis of the methylbenzyl group on the amino function. During both the hydrogenation and hydrogenolysis steps favorable stereoinduction was observed, and the products were obtained in 90-93% ee and 50-55% yield.

RX(1) OF 4



NOTE: stereoselective, optimized on cat., solvent, pressure and time,
 CON: high pressure
 18 hours, room temperature, 15 bar

RX(2) OF 4



NOTE: stereoselective, high pressure
 CON: 18 hours, room temperature, 15 bar

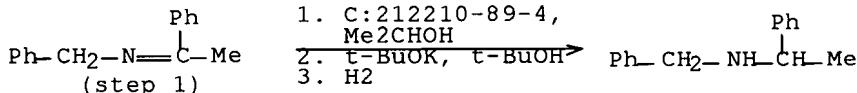
REFERENCE COUNT:

31

THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 20 OF 39 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 139:52500 CASREACT Full-text
TITLE: Enantioselective hydrogenation of imines using a
diverse library of ruthenium
dichloride(diphosphine)(diamine) precatalysts
AUTHOR(S): Cobley, Christopher J.; Henschke, Julian P.
CORPORATE SOURCE: Chirotech Technology Ltd., Cambridge, CB4 0WG, UK
SOURCE: Advanced Synthesis & Catalysis (2003), 345(1+2),
195-201
CODEN: ASCAF7; ISSN: 1615-4150
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A range of aromatic and cyclic imines were subjected to asym. hydrogenation with catalysts derived from complexes of the type RuCl₂(diphosphine)(diamine). Good to high enantioselectivities were observed For each imine, a library of chiral complexes based on different diphosphine and diamine combinations was screened. A different combination of diphosphine and diamine was required each time to obtain the optimum enantioselectivity.

RX (2) OF 8



NOTE: high pressure, optimization study, stereoselective
CON: STAGE {1} room temperature; room temperature
STAGE {2} room temperature; room temperature
STAGE {3} 18 - 21 hours, 50 - 65 deg C, 15 bar

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 21 OF 39 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 139:6955 CASREACT Full-text
TITLE: Application of Monodentate Secondary Phosphine Oxides,
a New Class of Chiral Ligands, in Ir(I)-Catalyzed
Asymmetric Imine Hydrogenation

AUTHOR(S): Jiang, Xiao-bin; Minnaard, Adriaan J.; Hessen, Bart; Feringa, Ben L.; Duchateau, Alexander L. L.; Andrien, Jean G. O.; Boogers, Jeroen A. F.; de Vries, Johannes G.

CORPORATE SOURCE: Department of Organic and Molecular Inorganic Chemistry, Stratingh Institute, University of Groningen, Groningen, 9747AG, Neth.

SOURCE: Organic Letters (2003), 5(9), 1503-1506
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English

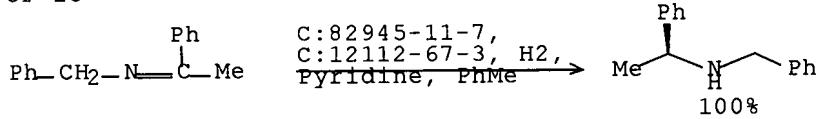
AB Secondary phosphine oxides hydrogenation. The synthesis

hydrolysis. They were obtained

HPLC. These new monodentate ligands were tested in the iridium-catalyzed hydrogenation of imines at 25 bar. Enantioselectivities up to 76% were obtained at $L/Ir = 2$. Addition of pyridine ($Pyr/Ir = 1:2$) raised the ee to 83%. Using pyridine as an additive allowed reduction of the L/Ir ratio to 1

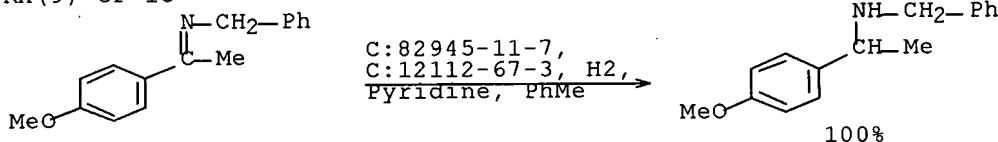
without reduction of ee. Thus, reaction of PhPCl₂ with t-BuMgBr followed by hydrolysis gave tert-butylphenylphosphine oxide which was used as cocatalyst for [Ir(COD)Cl]₂ catalyzed enantioselective hydrogenation of PhCMe:NCH₂Ph.

RX (8) OF 15



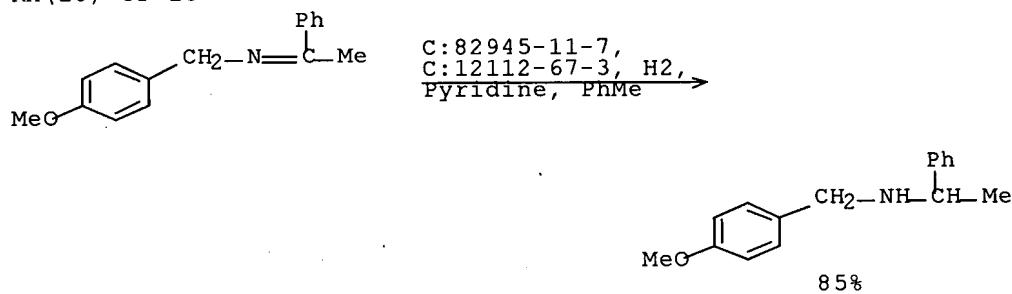
NOTE: stereoselective
CON: 24 hours, room temperature

RX (9) OF 15



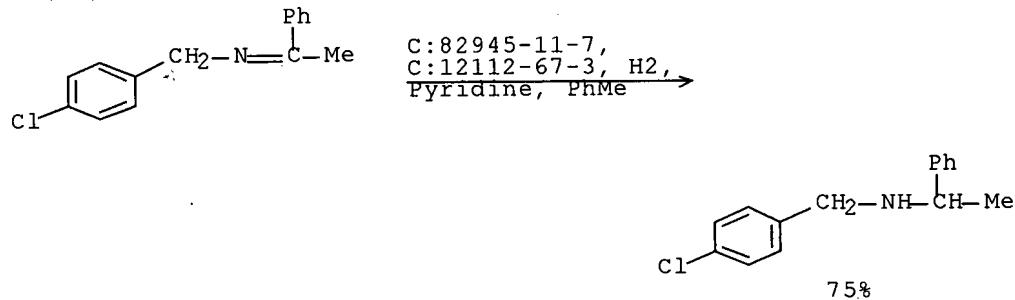
NOTE: stereoselective
CON: 24 hours, room temperature

RX (10) OF 15



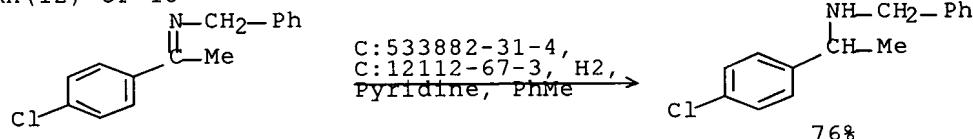
NOTE: stereoselective
CON: 24 hours, room temperature

RX (11) OF 15



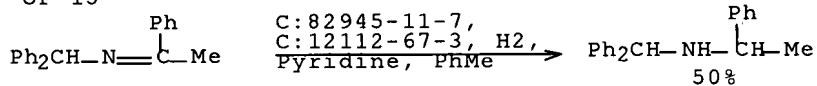
NOTE: stereoselective
CON: 24 hours, room temperature

RX (12) OF 15



NOTE: stereoselective
CON: 17 hours, room temperature

RX (14) OF 15

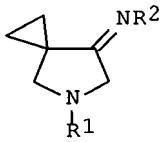
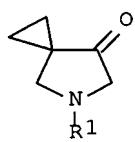
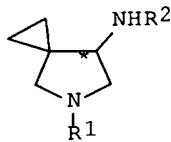


NOTE: stereoselective
CON: 48 hours, room temperature

REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

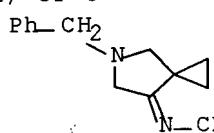
L26 ANSWER 22 OF 39 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 137:216865 CASREACT Full-text
 TITLE: Method for preparation of optically active 7-amino-5-azaspiro[2.4]heptane by imination of 7-oxo-5-azaspiro[2.4]heptane derivative and asymmetric hydrogenation of 7-imino-5-azaspiro[2.4]heptane derivative
 INVENTOR(S): Muto, Makoto; Nakayama, Takashi; Akiba, Toshifumi
 PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002255933	A	20020911	JP 2001-50384	20010226
PRIORITY APPLN. INFO.:			JP 2001-50384	20010226
OTHER SOURCE(S):		MARPAT 137:216865		
GI				

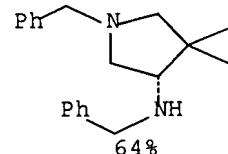


AB The title compound (I; R1 = R2 = H; * represents an asym. carbon) is prepared by condensation of 7-oxo-5-azaspiro[2.4]heptane derivative (II; R1 = H, amino-protecting group) with an amine of formula R2-NH2 (R2 = H, amino-protecting group) in the presence of an acid and reduction of the resulting imine (III; R1, R2 = same as above) in the presence of an asym. catalyst of formula MXmLn (M = group 8-10 transition metal; X ≠ H, halo, alkoxy, alkenyl; L = optically active phosphine ligand; m, n = an integer of 0-6) and optional deprotection of the resulting compound I (R1, R2 = H, amino-protecting group). This process gives in high yield the title compound of high optical purity which is useful as intermediate for antibacterial agents. Thus, to a solution of 1 g 5-benzyl-5-azaspiro[2.4]heptan-7-one and 642 mg benzylamine in benzene was added 0.1 mL Et2O.BF3 and the resulting mixture was refluxed with removal of water through a Dean-Stark trap to give 952 mg N-benzyl-N-(5-benzyl-5-azaspiro[2.4]hept-7-ylidene)amine (IV). (R)-2,2'-bis(di-p-tolylphosphino)-1,1'-binaphthyl (R-p-tol-BINAP) (67.9 mg) was added to a solution of 30.9 mg [Ir(COD)Cl]2 in 4.5 mL ethanol and stirred at room temperature for 2 h to give a catalyst solution which was added to an autoclave together with a solution of 290 mg IV in 4.5 mL ethanol and stirred at -10° under hydrogen pressure of 30 atm for 63 h to give 187 mg (S)-N-benzyl-N-(5-benzyl-5-azaspiro[2.4]heptan-7-yl)amine (V) (64% yield, 53% e.e.). To a suspension of 170 mg V and 17 mg 5% Pd-C in 2 mL toluene was added 0.58 mL concentrated HCl and stirred under hydrogen atmospheric for 5 h to give 177 mg 7-amino-5-azaspiro[2.4]heptane dihydrochloride (53% e.e.).

RX(1) OF 5

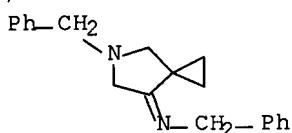


C:99646-28-3,
C:12112-67-3, H₂,
EtOH

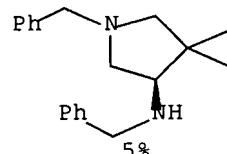


NOTE: high-pressure stereoselective (asym.) hydrogenation under hydrogen pressure of 30 atm at -10.degree. for 63 h; 54% e.e.

RX(3) OF 5

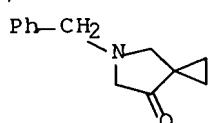


C:99646-28-3,
C:12112-67-3, H₂,
MeOH

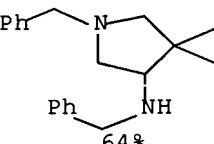


NOTE: high-pressure stereoselective (asym.) hydrogenation under hydrogen pressure of 30 atm at -10.degree. for 14 h; 76% e.e.

RX(4) OF 5 - 2 STEPS

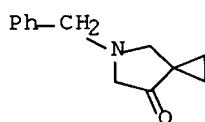


1. PhCH₂NH₂, BF₃-Et₂O,
Benzene
2. C:99646-28-3,
C:12112-67-3, H₂,
EtOH

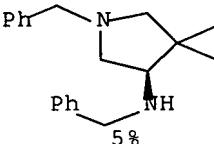


NOTE: 1) condensation (imination) under reflux with removal of water for 4 h, 2) high-pressure stereoselective (asym.) hydrogenation under hydrogen pressure of 30 atm at -10.degree. for 63 h; 54% e.e.

RX(5) OF 5 - 2 STEPS



1. PhCH₂NH₂, BF₃-Et₂O,
Benzene
2. C:99646-28-3,
C:12112-67-3, H₂,
MeOH



NOTE: 1) condensation (imination) under reflux with removal of water for 4 h, 2) high-pressure stereoselective (asym.) hydrogenation under hydrogen pressure of 30 atm at -10.degree. for 14 h; 76% e.e.

L26 ANSWER 23 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 136:150932 CASREACT Full-text

TITLE:

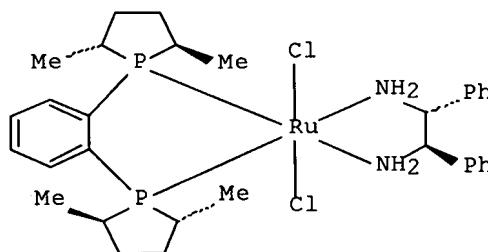
Ruthenium chiral diphosphine diamine complexes and their use in asymmetric hydrogenation for preparation of chiral amines

INVENTOR(S): Cobley, Christopher James; Henschke, Julian Paul; Ramsden, James Andrew

PATENT ASSIGNEE(S): Chirotech Technology Limited, UK
 SOURCE: PCT Int. Appl., 23 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008169	A1	20020131	WO 2001-GB3271	20010720
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2415738	A1	20020131	CA 2001-2415738	20010720
EP 1305278	A1	20030502	EP 2001-949777	20010720
EP 1305278	B1	20041103		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004504371	T	20040212	JP 2002-514079	20010720
US 2002095056	A1	20020718	US 2001-911059	20010723
US 6528687	B2	20030304		
PRIORITY APPLN. INFO.:				
			GB 2000-18146	20000724
			GB 2000-19227	20000804
			GB 2001-1458	20010119
			GB 2001-5742	20010308
			WO 2001-GB3271	20010720

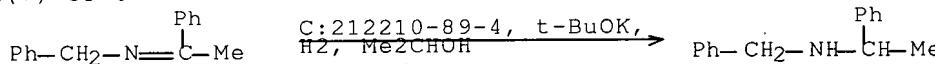
GI



AB A process is described for the preparation of an enantiomerically enriched chiral amine, $(R_1)(R_2)CNH(R_3)$, from an imine of formula $(R_1)(R_2)C:N(R_3)$ where (i) R_1 is aryl, R_2 is alkyl and R_3 is aryl or aryl-CH₂-, or (ii) R_2 is linked with R_1 and/or R_3 to form one or more rings and R_3 or R_1 (if not in a ring) is H or a noninterfering organic group, the number of C atoms in each of R_1 , R_2 and R_3 being up to 30, which comprises asym. hydrogenation of the imine in the presence of a base and, as catalyst, a ruthenium complex of a chiral diphosphine and a chiral diamine. Thus, $[(R,R)-Me-DuPHOS)RuCl_2((R,R)-DPEN)]$

(I) was prepared and used in the catalytic asym. hydrogenation of N-(1-phenylethylidene)aniline to give chiral phenyl(1-phenylethyl)amine in 85% ee.

RX(7) OF 8



NOTE: stereoselective, alternative catalysts gave lower selectivity

REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 24 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 136:102096 CASREACT Full-text

TITLE: Metal-Ligand Bifunctional Catalysis: A Nonclassical Mechanism for Asymmetric Hydrogen Transfer between Alcohols and Carbonyl Compounds

AUTHOR(S): Noyori, Ryoji; Yamakawa, Masashi; Hashiguchi, Shohei

CORPORATE SOURCE: Department of Chemistry and Research Center for Materials Science, Nagoya University, Chikusa, Nagoya, 464-8602, Japan

SOURCE: Journal of Organic Chemistry (2001), 66(24), 7931-7944
CODEN: JOCEAH; ISSN: 0022-3263

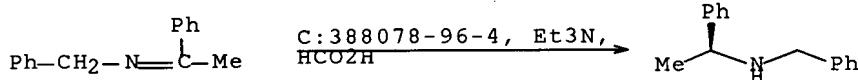
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Is substrate/metal complexation essential for hydrogenative saturation of unsatd. compds. No, it is not always necessary. The metal-ligand bifunctional mechanism allows for direct reduction of carbonyl compds. with an 18-electron transition metal hydride without C=O/metal interaction. Asym. transfer hydrogenation of aromatic carbonyl compounds using a 2-propanol/alkaline base system in the presence of RuCl[(S,S)-YCH(C₆H₅)CH(C₆H₅)NH₂](η₆-arene) (Y = O, NTs) or its analogs gives the corresponding S chiral alcs. of high enantiomeric purity. The reaction proceeds via a coordinatively saturated 18-electron complex, RuH[(S,S)-YCH(C₆H₅)CH(C₆H₅)NH₂]-(η₆-arene). The hydridic RuH and protic NH are simultaneously delivered to a C=O linkage via a six-membered pericyclic mechanism, giving an S alc. and RuH[(S,S)-YCH(C₆H₅)CH(C₆H₅)NH₂]-(η₆-arene). The latter 16-electron Ru amide complex dehydrogenates 2-propanol to regenerate the Ru hydride species. A formic acid/triethylamine mixt.formic acid/triethylamine mixture serves as a better reducing agent. The recognition of carbonyl enantiofaces in the hydrogen transfer is made largely by the attractive CH/π interaction between the η₆-arene ligand and the aromatic substituent in carbonyl substrates.

RX(12) OF 13



NOTE: stereoselective

REFERENCE COUNT:

158 THERE ARE 158 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 25 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 134:280422 CASREACT Full-text

TITLE: Stoichiometric, Catalytic, and Enantioface-Selective Hydrogenation of C:N Bonds by an Ionic Mechanism

AUTHOR(S): Magee, Matthew P.; Norton, Jack R.

CORPORATE SOURCE: Department of Chemistry, Columbia University, New York, NY, 10027, USA

SOURCE: Journal of the American Chemical Society (2001), 123(8), 1778-1779

CODEN: JACSAT; ISSN: 0002-7863

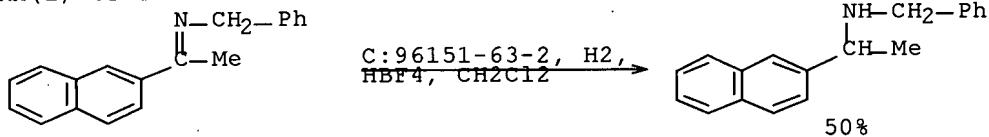
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

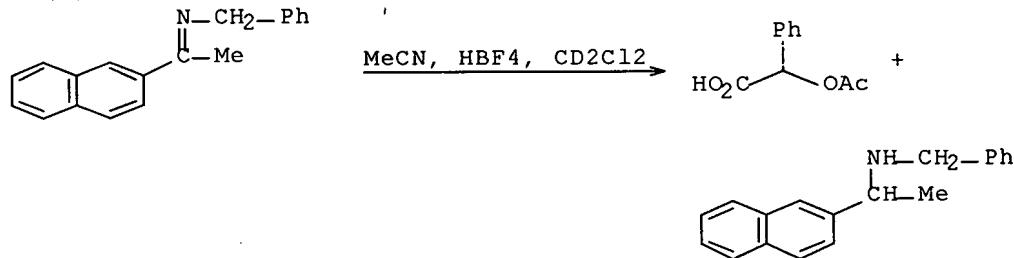
LANGUAGE: English

AB The authors report the asym. hydrogenation of tetra-alkyl-substituted C:N cations using piano-stool chiral bisphosphine cyclopentadienylruthenium hydride complex catalysts. The mechanism of these reaction were discussed. Catalytic ionic hydrogenation can be done in an ionizing solvent and new catalysts screened easily by determining the enantioselectivity of stoichiometric hydride transfer.

RX(1) OF 11



RX (2) OF 11



REFERENCE COUNT:

26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 26 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 132:165934 CASREACT Full-text

TITLE: Method for preparation of optical active benzylamines by stereoselective hydrogenation of ketone N-benzylimines

INVENTOR(S): Ikehira, Hideyuki

PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT: 1

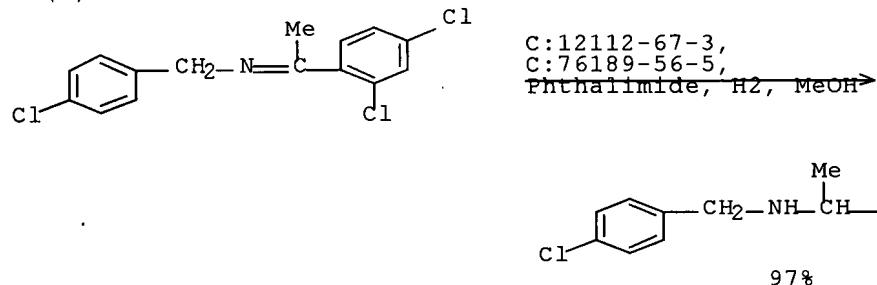
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000053618	A	20000222	JP 1998-220661	19980804
PRIORITY APPLN. INFO.:			JP 1998-220661	19980804

OTHER SOURCE(S): MARPAT 132:165934

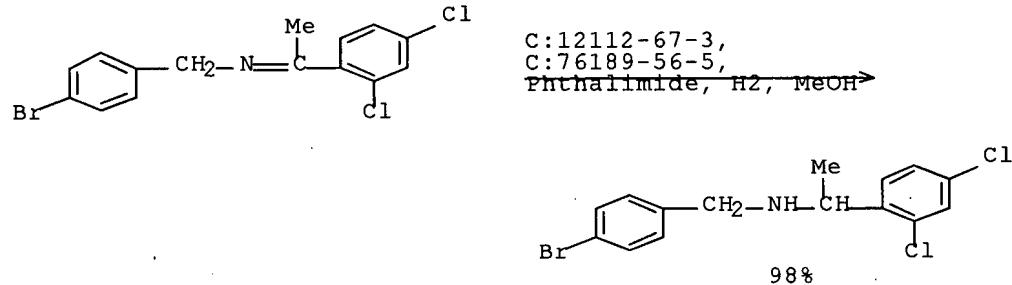
AB The title compds. represented by formula R1R2CHNHCH2R3 [R1, R2 = H, halo, (un)substituted alkyl, aralkyl, aryl, alkenyl, or alkoxy, aryloxy, alkoxy carbonyl; or R1 and R2 are linked to each other to form a cyclic compound; R3 = p-halophenyl] are prepared by hydrogenation of ketone N-benzylimines represented by formula R1R2C:NCH2R3 (R1 - R3 = same as above) in the presence of a group VIII transition metal complex and an optically active phosphine compound. Thus, 21.5 mg [IrCl(cod)]2, 39.9 (S)-BINAP, and 18.8 mg phthalimide were added to a solution of 200 mg N-[1-(2,4-dichlorophenyl)ethylidene]-p-chlorobenzylamine in 5 mL MeOH in an autoclave and stirred under 50 atm H pressure at 30° for 18 h to give 96.9% N-[1-(2,4-dichlorophenyl)ethyl]-p-chlorobenzylamine (70% ee).

RX(1) OF 5



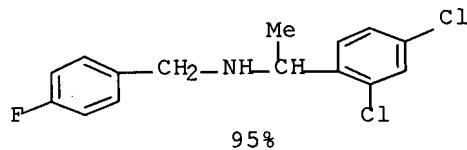
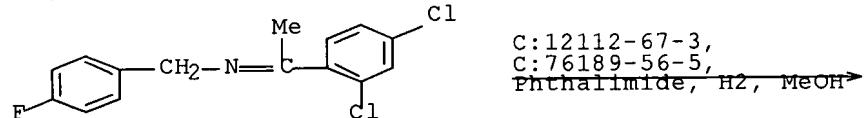
NOTE: asym. hydrogenation; 70% ee; 50 atm hydrogen pressure and 30. degree. for 18 h

RX(2) OF 5



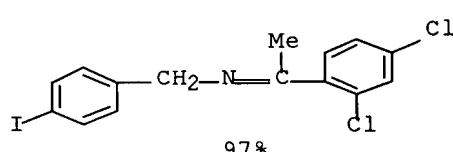
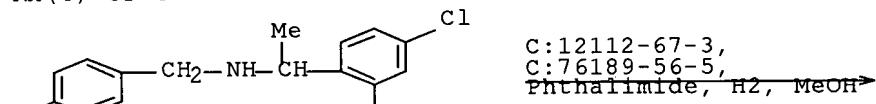
NOTE: asym. hydrogenation; 67% ee; 50 atm hydrogen pressure and 30. degree. for 18 h

RX (3) OF 5



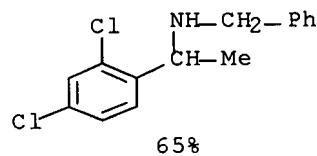
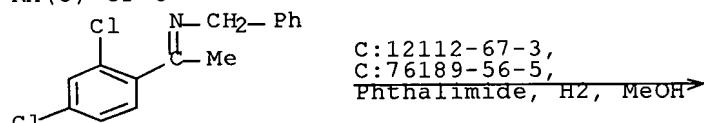
NOTE: asym. hydrogenation; 68% ee; 50 atm hydrogen pressure and 30. degree. for 18 h

RX (4) OF 5



NOTE: asym. hydrogenation; 62% ee; 50 atm hydrogen pressure and 30. degree. for 18 h

RX (5) OF 5

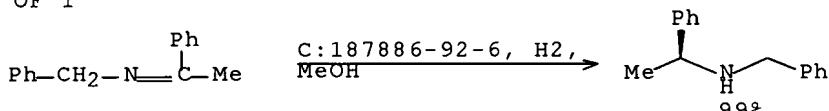


NOTE: asym. hydrogenation; 15% ee; 50 atm hydrogen pressure and 30. degree. for 18 h

AUTHOR(S): Tararov, Vitali I.; Kadyrov, Renat; Riermeier, Thomas H.; Holz, Jens; Borner, Armin
 CORPORATE SOURCE: Institut fur Organische Katalyseforschung an der Universitat Rostock e.V., Rostock, D-18055, Germany
 SOURCE: Tetrahedron: Asymmetry (1999), 10(20), 4009-4015
 CODEN: TASYE3; ISSN: 0957-4166
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The asym. hydrogenation of N-(1-phenylethyldene)benzylamine with a range of Rh(I)-diphosphine and diphosphinite catalysts was studied. The reaction is strongly sensitive to the size of the metal chelate. Complexes based on five- and six-membered chelates or electron-rich alkylphosphines gave poor or moderate conversions. The reactivity of diphosphine catalysts could be increased by the addition of p-toluenesulfonic acid. Unexpectedly, Rh-complexes based on chiral diphosphinites and a diphosphite also rapidly converted the substrate to the desired amine. Highest efficiency was observed with a Rh(I) complex with (R,R)-1,2-cyclohexanol-bisdiphenylphosphinite [(R,R)-bdpcch] as chiral ligand. Without any additive complete hydrogenation of the imine was achieved within 5 h. The product was produced in an enantioselectivity of 71%.

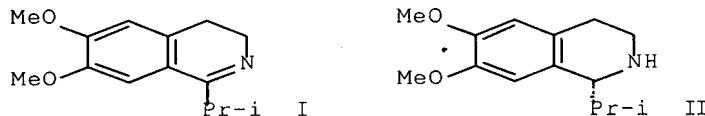
RX (1) OF 1



NOTE: stereoselective

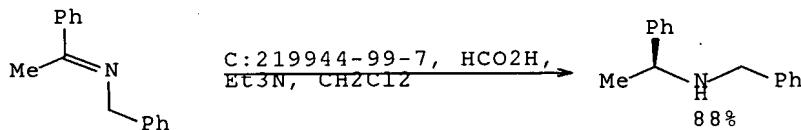
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 28 OF 39 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 131:299536 CASREACT Full-text
 TITLE: A Chiral Rhodium Complex for Rapid Asymmetric Transfer Hydrogenation of Imines with High Enantioselectivity
 AUTHOR(S): Mao, Jianmin; Baker, David C.
 CORPORATE SOURCE: Department of Chemistry, The University of Tennessee, Knoxville, TN, 37996-1600, USA
 SOURCE: Organic Letters (1999), 1(6), 841-843
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB A chiral Rh complex, (R)-Cp^{*}RhCl[(1S,2S)-p-TsNCHPhCHPhNH₂] (1a, (S,S)-Cp^{*}RhClTsDPEN), generated from [Cp^{*}RhCl₂]₂ and (1S,2S)-N-p-toluenesulfonyl-1,2-diphenylethylenediamine [(S,S)-TsDPEN], and its enantiomer 1b provide superior catalysts for the rapid, high-yielding, asym. transfer hydrogenation of some heterocyclic imines, using an HCO₂H-Et₃N azeotrope as the H source. For example, dihydroisoquinoline I underwent asym. hydrogenation to give 96% tetrahydroisoquinoline (R)-II (99% ee) when the hydrogenation was conducted at a substrate/catalyst (S/C) molar ratio of 200:1 using a 5:2 formic acid-triethylamine azeotrope as the hydrogen source and the isolated crystalline complex 1a as catalyst in CH₂Cl₂ at 20° for 10 min. When the catalyst 1b was formed in situ prior to hydrogen, equivalent results were obtained. The catalysts were well behaved in a range of solvents, both protic and aprotic; however, the reactions gave slightly better enantioselectivity in polar solvents. Complex 1b was characterized by single-crystal x-ray diffraction anal.

RX (3) OF 5



NOTE: stereoselective, 8.4% ee , 20.degree., 10 min

REFERENCE COUNT:

38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 29 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 131:184719 CASREACT Full-text

TITLE: Iridium-Catalyzed Enantioselective Hydrogenation of Imines in Supercritical Carbon Dioxide

AUTHOR(S): Kainz, Sabine; Brinkmann, Axel; Leitner, Walter; Pfaltz, Andreas

CORPORATE SOURCE: Max-Planck-Institut fuer Kohlenforschung, Muelheim/Ruhr, 45470, Germany

SOURCE: Journal of the American Chemical Society (1999), 121(27), 6421-6429
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

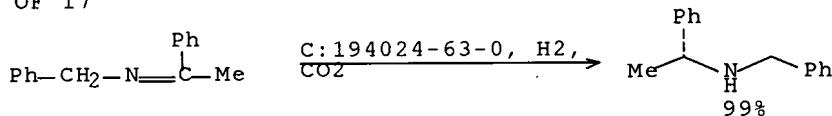
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Supercrit. carbon dioxide (scCO₂) was shown to be a reaction medium with unique properties for highly efficient iridium-catalyzed enantioselective hydrogenation of prochiral imines. Cationic iridium(I) complexes with chiral phosphinodihydrooxazoles, modified with perfluoroalkyl groups in the ligand or in the anion, were synthesized and tested in the hydrogenation of N-(1-phenylethylidene)aniline. Both the side chains and the lipophilic anions increased the solubility, but the choice of the anion also had a dramatic effect on the enantioselectivity with tetrakis-3,5-bis(trifluoromethyl)phenylborate (BARF) leading to the highest asym. induction. (R)-N-phenyl-1-phenylethylamine was formed quant. within 1 h in

scCO_2 [$d(\text{CO}_2) = 0.75 \text{ g mL}^{-1}$] at 40° and a H_2 pressure of 30 bar with enantiomeric excesses of up to 81% using 0.078 mol % catalyst. The use of scCO_2 instead of conventional solvents such as CH_2Cl_2 allowed the catalyst loading to be lowered significantly owing to a change in the rate profile of the reaction. The homogeneous nature of the catalytically active species under the reaction conditions was demonstrated and was found to depend strongly on the composition of the reaction mixture and especially on the presence of the substrate. Utilizing the selective extractive properties of scCO_2 , the product could be readily separated from the catalyst, which could be recycled several times without significant loss of activity and enantioselectivity. High-pressure FT-IR and NMR investigations revealed that the reactivity of the products to form the corresponding carbamic acids plays an important role for the application of this new methodol.

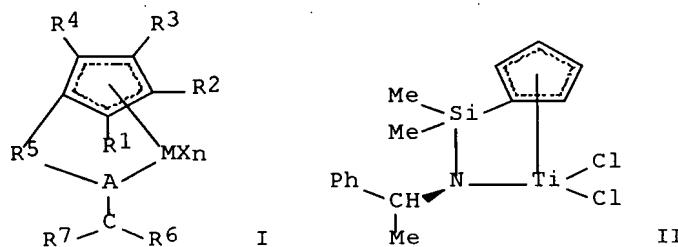
RX (3) OF 17



NOTE: stereoselective, supercrit. CO₂/solvent, high pressure

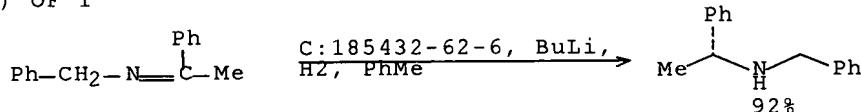
REFERENCE COUNT: 81 THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19622271 A1		19971204	DE 1996-19622271	19960603
OTHER SOURCE(S):		MARPAT 128:89013		
GI				



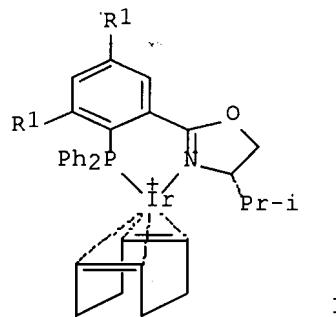
AB Chiral title compds. of the general formula I wherein M can represents Ti, Zr, Hf, V, Nb, Ta or an element of the Lanthanide series, X can represents halogen, H or alkyl or aryl group, R1-R4 can represent H, alkyl, cycloalkyl or organosilyl group, R5 can represents Si-, Ge-, Sn-, B-, Al-containing group, O or S, A represents B, Al, Ga, In, Tl, N, P, As, Sb, and R6 and R7 can represent C1-C10 alkyl, aryl or cycloalkyl or heteroatom groups. E.g., titanium complex II was prepared from [(chlorodimethylsilyl)cyclopentadienyl]titanium trichloride and lithium (1R)-1-phenylethyl amide in the presence of Et₃N/THF/Et₂O at -78° in 72% yield; PhCH₂N:CM₂Ph was hydrogenated under 150 bar of H₂ in the presence of catalyst II (which had been pretreated with BuLi in toluene) to give a 92% yield of (1R)-N-benzyl-1-phenylethylamine.

RX (1) OF 1

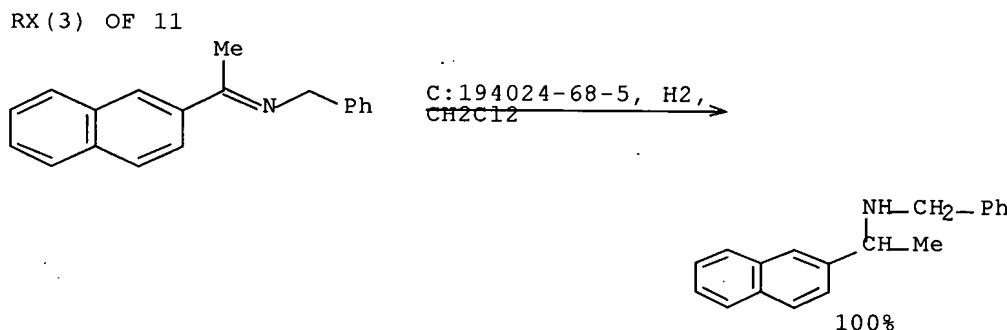
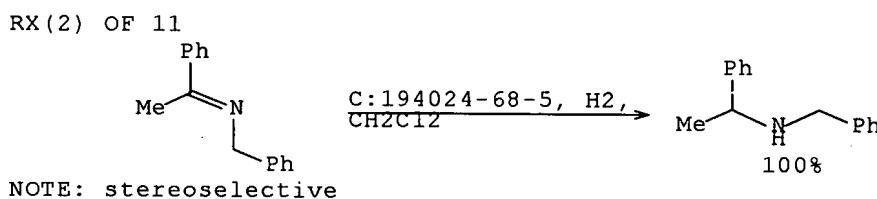


NOTE: stereoselective

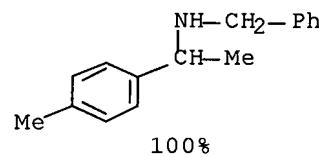
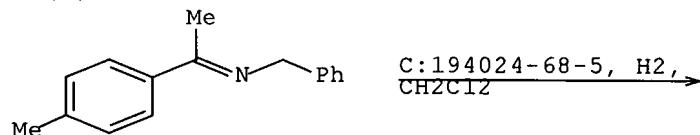
L26 ANSWER 31 OF 39 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 127:176221 CASREACT Full-text
 TITLE: Enantioselective hydrogenation of imines with chiral (phosphanodihydrooxazole)iridium catalysts
 AUTHOR(S): Schnider, Patrick; Koch, Guido; Pretot, Roger; Wang, Guozhi; Bohnen, Frank Michael; Kruger, Carl; Pfaltz, Andreas
 CORPORATE SOURCE: Institut Organische Chemie, Universitat Basel, Basel, CH-4056, Switz.
 SOURCE: Chemistry--A European Journal (1997), 3(6), 887-892
 CODEN: CEUJED; ISSN: 0947-6539
 PUBLISHER: Wiley-VCH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Cationic iridium(I) complexes I ($R_1 = H, Me$) were prepared and used as catalysts for the enantioselective hydrogenation of prochiral N-alkyl and N-aryl imines. The complexes are air-stable crystalline solids that can be readily prepared and are easy to handle. The structures of two complexes are determined by X-ray anal. For N-alkyl imines of acetophenone, enantiomeric excesses of up to 79% were obtained. Dialkyl ketimines and cyclic imines showed lower reactivity and selectivity. A remarkable dilution effect was observed for the hydrogenation of the N-Ph imine of acetophenone: decreasing the substrate and catalyst concentration led to a significant improvement of the enantioselectivity. Thus, up to 89% ee could be achieved using 0.1 mol% of catalyst. The highest enantioselectivities were obtained in weakly coordinating solvents such as CH_2Cl_2 . Additives were found to poison the catalyst. Hydrogen pressures of 100 bar were usually employed, but in some cases identical results were achieved with only 1 bar H_2 .

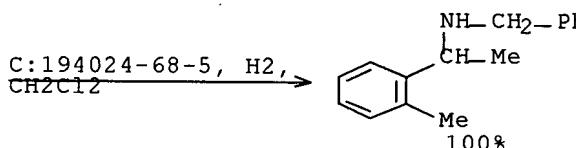
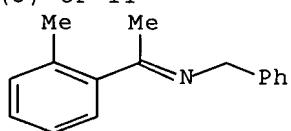


RX (4) OF 11



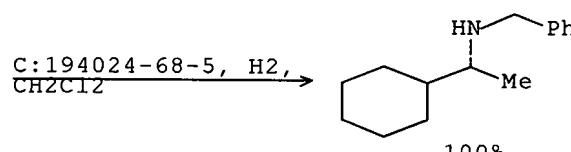
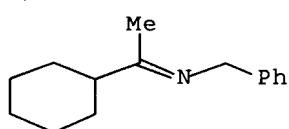
NOTE: stereoselective

RX (5) OF 11



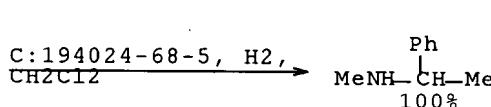
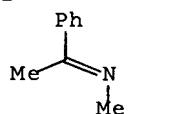
NOTE: stereoselective

RX (6) OF 11



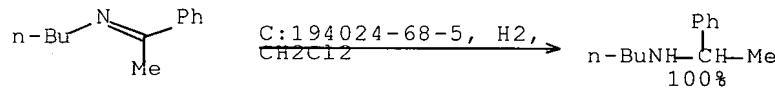
NOTE: stereoselective

RX (7) OF 11

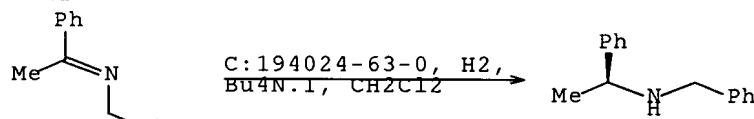


NOTE: stereoselective

RX(8) OF 11



RX(11) OF 11



NOTE: adding iodide reversed the configuration of the product

REFERENCE COUNT:

53

THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 32 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 126:293447 CASREACT Full-text

TITLE: Process for the preparation of optically active 1-aminophosphonic acid derivatives and novel phosphonate compounds

INVENTOR(S): Shibasaki, Masakatsu; Sasai, Hiroaki; Tahara, Yoshihiro

PATENT ASSIGNEE(S): Hokko Chemical Industry Co., Ltd., Japan

SOURCE: PCT Int. Appl., 69 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

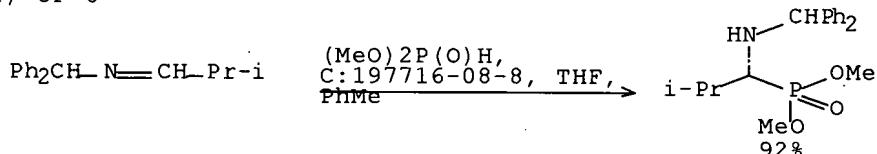
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9711954	A1	19970403	WO 1996-JP2794	19960926
W: US				
RW: CH, DE, FR, GB				
JP 09151191	A	19970610	JP 1996-255195	19960926
JP 3574715	B2	20041006		
EP 877028	A1	19981111	EP 1996-932010	19960926
EP 877028	B1	20040825		
R: CH, DE, FR, GB, LI				
US 6084123	A	20000704	US 1998-43678	19980520
JP 2004337855	A	20041202	JP 2004-168628	20040607
PRIORITY APPLN. INFO.:				
			JP 1995-248044	19950926
			JP 1996-255195	19960926
			WO 1996-JP2794	19960926
OTHER SOURCE(S):	MARPAT 126:293447			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Characterized is a process for the preparation of optically active (R)- or (S)-1-aminophosphonic acid derivs. (I or II; R₂ = alkyl, cycloalkyl, etc.), which comprises reacting an N-blocked imine R₂N:CHR₁ (R₂ = same as above; R₁ = Ph₂CH, alkoxyphenyl) with a phosphonic ester in the presence of an asym. catalyst and subjecting the intermediate to deblocking through hydrogenation and acidic hydrolysis. A process for the preparation of an asym. catalyst comprising a rare earth element-alkali metal-binaphthol complex to form an (R)- or (S)-N-blocked-1-aminophosphonate compound is also claimed. Thus, Ph₂CHN:CHMe₂ was reacted with (MeO)₂P(O)H in the presence of catalyst (R)-La-K-B complex (III) at 20° for 56 h and followed by hydrogenation and acidic hydrolysis to give I (R₂ = CHMe₂).

RX(1) OF 6



NOTE: 20.degree. for 56 h

L26 ANSWER 33 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 123:227944 CASREACT Full-text

TITLE:

Asymmetric reactions catalyzed by chiral metal complexes. LXII. Efficient asymmetric hydrogenation of imines catalyzed by a neutral iridium(I) complex of (4R,5R)-MOD-DIOP

AUTHOR(S): Morimoto, Toshiaki; Nakajima, Noriya; Achiwa, Kazuo
CORPORATE SOURCE: Sch. Pharmaceutical Sciences., Univ. Shizuoka, Shizuoka-shi, 422, Japan

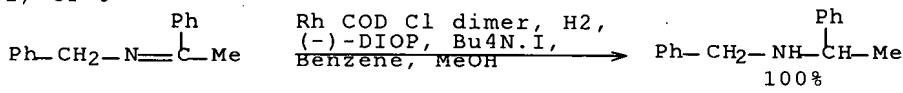
SOURCE: Chemical & Pharmaceutical Bulletin (1994), 42(9), 1951-3

PUBLISHER: CODEN: CPBTAL; ISSN: 0009-2363
Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal
LANGUAGE: English

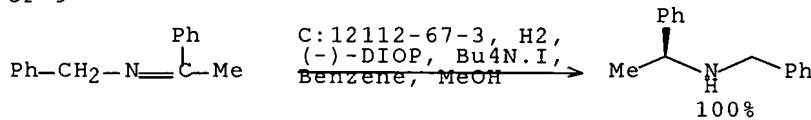
AB A neutral iridium(I) complex of (4R,5R)-MOD-DIOP (I) was found to be an efficient catalyst for the asym. hydrogenation of imines, N-(α -methylbenzylidene)benzylamine and 2,3,3-trimethylindolenine, in the presence of tetrabutylammonium iodide. A high enantioselectivity with up to 81.4% ee was achieved. Reduction of 2,3,3-trimethyl-3H-indole with I and di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]diiridium gave (+)-2,3-dihydro-2,3,3-trimethyl-1H-indole (66.2% enantiomeric excess).

RX(1) OF 9



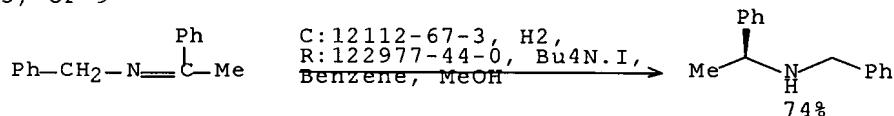
NOTE: STEREOSELECTIVE

RX (2) OF 9



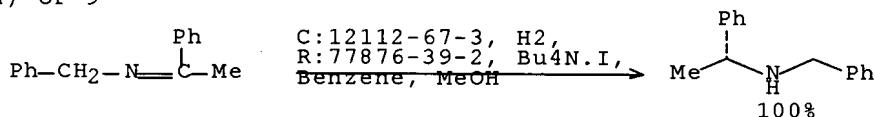
NOTE: STEREOSELECTIVE

RX (3) OF 9



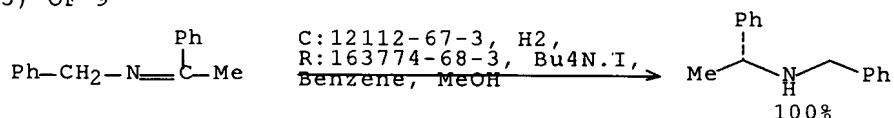
NOTE: STEREOSELECTIVE

RX (4) OF 9



NOTE: STEREOSELECTIVE

RX (5) OF 9



NOTE: STEREOSELECTIVE

L26 ANSWER 34 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 122:80569 CASREACT Full-textTITLE: Catalytic Asymmetric Hydrogenation of Imines
with a Chiral Titanocene Catalyst: Kinetic and Mechanistic Investigations

AUTHOR(S): Willoughby, Christopher A.; Buchwald, Stephen L.

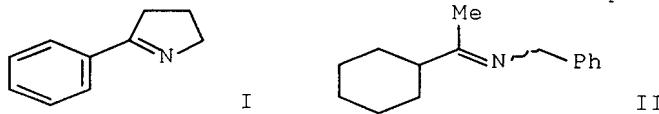
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SOURCE: Journal of the American Chemical Society (1994),

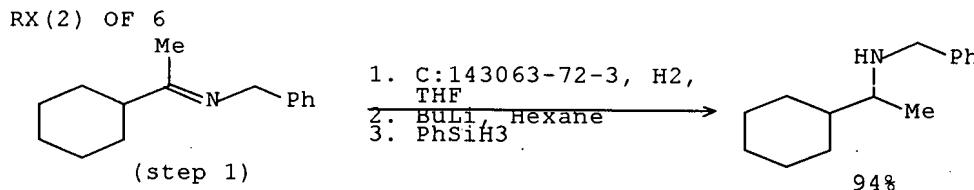
116(26), 11703-14
 CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER:
 DOCUMENT TYPE:
 LANGUAGE:
 GI

American Chemical Society
 Journal
 English



AB A kinetic study of the asym. titanocene-catalyzed imine hydrogenation has revealed the rate law to be rate = $k_{obs}[Ti][H_2]$, for cyclic imine (I) and acyclic imine (II). This rate law is consistent with a mechanism in which the imine reacts with a titanium hydride in a fast 1,2-insertion step, to form a titanium amide intermediate, followed by slow reaction of the amide complex with hydrogen to produce the amine and regenerate the titanium hydride. Labeling studies for the hydrogenation of I and studies using enantiomerically enriched aldimine 6 indicate that β -H elimination is also slow, relative to hydrogenolysis, for both I and II. The enantiomeric excesses for the hydrogenation of I were essentially insensitive to changes in reaction conditions. However, for II, the ee's were dependent on several variables, most significantly hydrogen pressure. This phenomenon has been explained on the basis of the interconversion of the syn and anti isomers of II during the hydrogenation. It has been shown that syn-II reacts faster than anti-II, a necessary condition for the explanation presented to hold true. A stereochem. model based on steric and electronic considerations has been proposed to account for the observed selectivity. This model can aid in predicting the absolute configurations of the amines formed in this process.



NOTE: STEREOSELECTIVE, SELECTIVITY DIMINISHES WITH LOWER HYDROGENATION PRESSURE, STARTING MATERIAL IS 11:1 E:Z ISOMERS

TITLE: Catalytic asymmetric and non-asymmetric reduction of imines and oximes using metal catalysts

INVENTOR(S): Buchwald, Stephen L.; Willoughby, Christopher A.

PATENT ASSIGNEE(S): Massachusetts Institute of Technology, USA

SOURCE: U.S., 10 pp. Cont.-in-part of U.S. Ser. No. 698,940, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 8

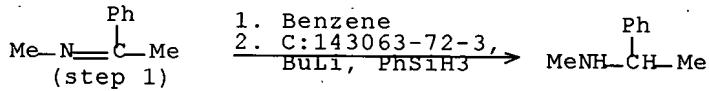
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5292893	A	19940308	US 1991-792229	19911114
US 5286878	A	19940215	US 1990-616892	19901121
CA 2096747	A1	19920522	CA 1991-2096747	19911121
WO 9209545	A2	19920611	WO 1991-US8738	19911121
WO 9209545	A3	19921029		
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
EP 558656	A1	19930908	EP 1992-901632	19911121
EP 558656	B1	19960417		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 06502867	T	19940331	JP 1992-502333	19911121
AT 136878	T	19960515	AT 1992-901632	19911121
US 5442119	A	19950815	US 1993-90338	19930712
US 5489682	A	19960206	US 1994-195358	19940210
PRIORITY APPLN. INFO.:			US 1990-616892	19901121
			US 1991-698940	19910513
			US 1991-698939	19910513
			US 1991-749111	19910823
			US 1991-792227	19911114
			US 1991-792229	19911114
			US 1991-792233	19911114
			WO 1991-US8738	19911121
			US 1993-90338	19930712

OTHER SOURCE(S): MARPAT 120:322918

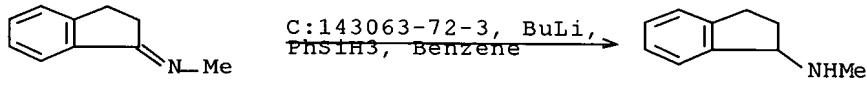
AB The catalytic asym. reduction of imines [e.g., PhC(:NMe)Me], oximes, and hydrazones using chiral catalysts [e.g., (R,R)-ethylene-1,2-bis(η 5-4,5,6,7-tetrahydroindenyl)titanium (R)-1,1'-binaphth-2,2'diolate], to chiral amines (e.g., N-methyl-1-phenylethylamine) is described where the reduction is carried out in the presence of an inert gas or in a H atmospheric, where H is the stoichiometric reducing agent (i.e., hydrogenation).

RX(1) OF 4



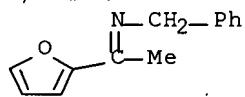
NOTE: stereoselective

RX(2) OF 4



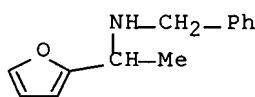
NOTE: stereoselective

RX (3) OF 4



C:143063-72-3, BuLi,

PhSiH3, THF, Hexane



NOTE: stereoselective

L26 ANSWER 36 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 119:8408 CASREACT Full-text

TITLE: Diastereoselective hydrogenation and kinetic resolution of imines using rhodium/diphosphine catalyzed hydrogenation

AUTHOR(S): Lensink, Cornelis; De Vries, Johannes G.

CORPORATE SOURCE: Dep. Chem. Prod. - Intermed., DSM Res., Geleen, 6160 MD, Neth.

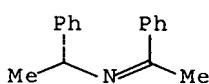
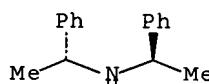
SOURCE: Tetrahedron: Asymmetry (1993), 4(2), 215-22
CODEN: TASYE3; ISSN: 0957-4166

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Kinetic resolution of racemic α -methylbenzylamine can be achieved with 98% e.e. of the remaining amine at 70% conversion using the Rhodium/2S,4S-BDPP catalyzed asym. hydrogenation of imines. The same catalyst will hydrogenate optically pure α -methylbenzylamines with a diastereoselectivity of up to 333:1.

RX (1) OF 1

C:77876-39-2,
Rh COD Cl dimer,
MeOH

NOTE: stereoselective

L26 ANSWER 37 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 110:192328 CASREACT Full-text

TITLE: Rhodium(I)-catalyzed asymmetric hydrogenation of imines

AUTHOR(S): Kang, Guo Jun; Cullen, William R.; Fryzuk, Michael D.; James, Brian R.; Kutney, James P.

CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.

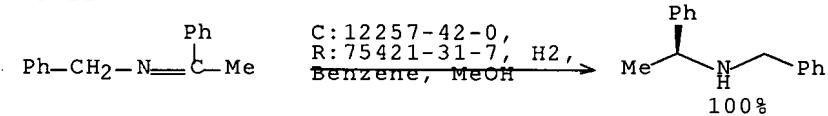
SOURCE: Journal of the Chemical Society, Chemical Communications (1988), (22), 1466-7
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

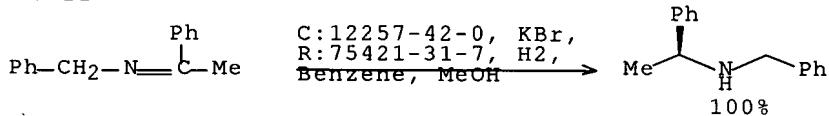
AB High-pressure hydrogenation of $\text{RC}_6\text{H}_4\text{CMe:NCH}_2\text{Ph}$ ($\text{R} = \text{H}$, o- and p-MeO) in the presence of a catalyst prepared from chloronorbornadienylrhodium dimer and $(\text{R})-(+)-\text{Ph}_2\text{PCHR}1\text{CH}_2\text{PPh}_2$ ($\text{R}1 = \text{cyclohexyl}$) in 1:1 $\text{C}_6\text{H}_6\text{-MeOH}$ containing KI gave 90-100% (S)- $\text{RC}_6\text{H}_4\text{CHMeNHCH}_2\text{Ph}$ in 60-91% enantiomeric excess.

RX (1) OF 11



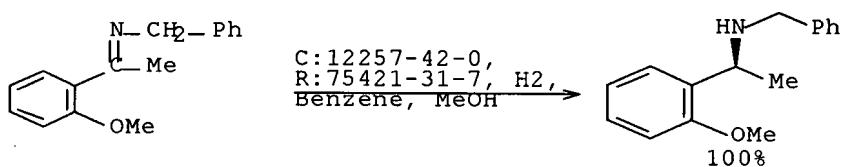
NOTE: high pressure

RX (2) OF 11



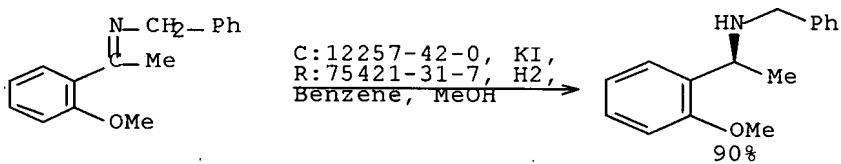
NOTE: high pressure

RX (3) OF 11



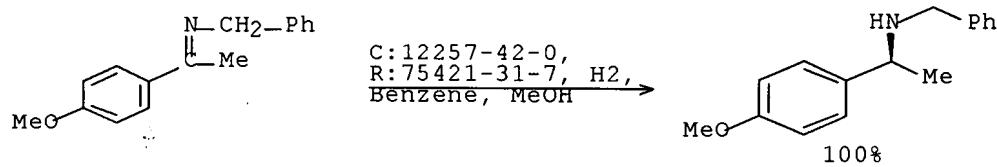
NOTE: high pressure

RX (4) OF 11



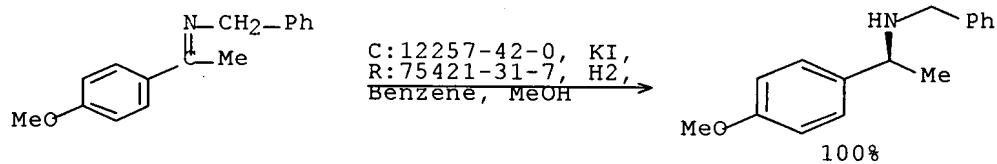
NOTE: high pressure

RX (5) OF 11



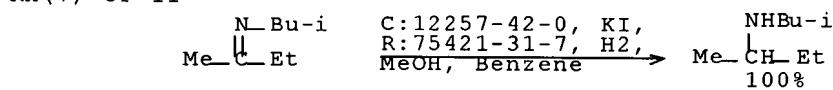
NOTE: high pressure

RX (6) OF 11



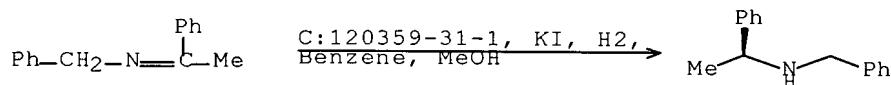
NOTE: high pressure

RX (7) OF 11

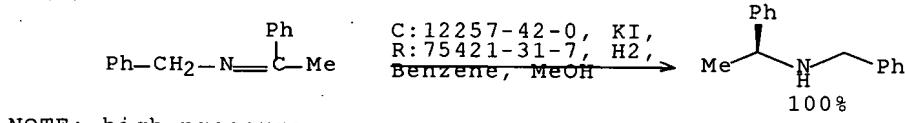


NOTE: high pressure

RX (8) OF 11



RX (9) OF 11



NOTE: high pressure

ACCESSION NUMBER:

102:204036 CASREACT Full-text

TITLE:

A facile method for the preparation of
2,4-bis(diphenylphosphino)pentane (BDPP) enantiomers
and their application in asymmetric
hydrogenation

AUTHOR(S):

Bakos, Jozsef; Toth, Imre; Heil, Balint; Marko, Laszlo
Inst. Org. Chem., Univ. Chem. Eng., Veszprem, H-8201,
Hung.

CORPORATE SOURCE:

Journal of Organometallic Chemistry (1985), 279(1-2),
23-9

SOURCE:

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE:

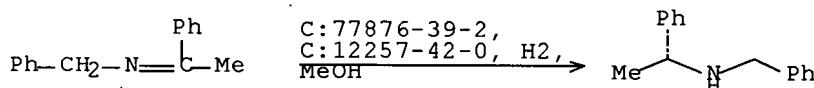
Journal

LANGUAGE:

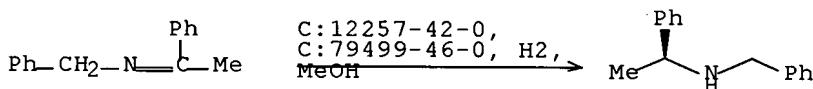
English

AB Asym. heterogeneous hydrogenation of acetylacetone was applied for the preparation of both enantiomers (2R,4R and 2S,4S) of 2,4-bis(diphenylphosphino)pentane (BDPP). Among the chiral phosphines prepared up to now BDPP appears to be unique in the sense that its rhodium(I) complexes serve as effective homogeneous asym. hydrogenation catalysts not only for the reduction of Z- α -amidoacrylic acids but also for the reduction of α -ethylstyrene, acetophenone, and acetophenone benzylimine. The analogous phosphinite ligand BDPOP [2,4-bis[(diphenylphosphinyl)oxy]pentane] yields a less selective catalyst.

RX (26) OF 31



RX (27) OF 31



L26 ANSWER 39 OF 39 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 78:110112 CASREACT Full-text

TITLE:

Asymmetric hydrogenation of the C=N bond.
Factors controlling the stereoselectivity

AUTHOR(S):

Yoshida, Takao; Harada, Kaoru

CORPORATE SOURCE:

Fac. Sci., Osaka Univ., Toyonaka, Japan

SOURCE:

Bulletin of the Chemical Society of Japan (1972),
45(12), 3706-10

CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE:

Journal

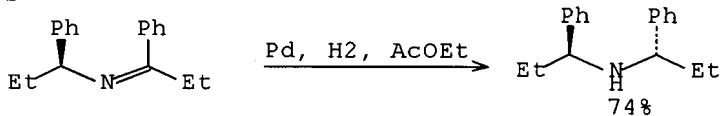
LANGUAGE:

English

AB Asym. catalytic hydrogenation of Schiff bases, i.e., N-(methylbenzylidene)- α -methylbenzylamine (I) and N-(ethylbenzylidene)- α -ethylbenzylamine (II) using 10% Pd(OH)₂/C was studied to elucidate the steric course of the reaction. Effects of temperature, solvent, pressure, the amount of the catalyst, and ratio of the syn and anti isomers on the asym. hydrogenation were investigated. Temperature, solvent, and the amount of the catalyst were factors which controlled the stereoselectivity of the reaction. The hydrogenation of I always gave a higher asym. yield than that of II. Lower

temperature, lower polarity of the solvent, and decreased amount of catalyst gave higher stereoselectivities in the hydrogenation reactions.

RX(1) OF 1

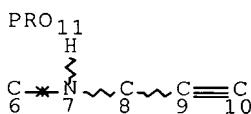
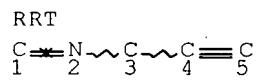


NOTE: Classification: Hydrogenation; Diastereoselective; Reduction; #
Conditions: H2 Pd(OH)2-C; EtOAc; # Comments: reactant has (S) (-) configuration; product has (S,S) (-) configuration

=> d que 130

L27

STR



NODE ATTRIBUTES:

NSPEC IS RC AT 1
NSPEC IS RC AT 6

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

*****MAPPINGS*****

NOD	SYM	ROL	NOD	SYM	ROL
2	N	RRT	7	N	PRO
4	C	RRT	9	C	PRO
7	N	PRO	2	N	RRT
9	C	PRO	4	C	RRT

L29 10 SEA FILE=CASREACT SSS FUL L27 (12 REACTIONS)
L30 10 SEA FILE=CASREACT ABB=ON PLU=ON L29/COM

=> d 130 ibib abs crd tot

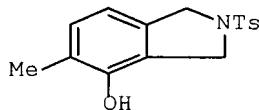
L30 ANSWER 1 OF 10 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 146:401767 CASREACT Full-text

TITLE: Heterogeneous gold-catalyzed synthesis of phenols
AUTHOR(S): Carrettin, Silvio; Blanco, M. Carmen; Corma, Avelino;
Hashmi, A. Stephen K.

CORPORATE SOURCE: Instituto de Tecnologia Quimica, UPV-CSIC, Universidad

SOURCE:

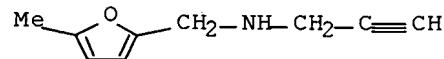
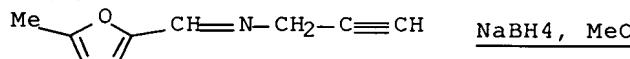
Politecnica de Valencia, Valencia, Spain
 Advanced Synthesis & Catalysis (2006), 348(10+11),
 1283-1288
 CODEN: ASCAF7; ISSN: 1615-4150
 Wiley-VCH Verlag GmbH & Co. KGaA
 Journal
 English
 GI



I

AB Nanoparticles of gold supported on nanocryst. CeO₂ catalyze the isomerization of ω -alkynylfurans to phenols, e.g., I. Initial leaching of gold was observed, which could be minimized by calcining. Subsequent runs showed that once all soluble species had leached, the surface-bound, cationic gold species is still active and can reach turnover nos. of up to 391. This is the first time that a heterogeneous gold catalyst showed activity in gold-catalyzed phenol synthesis.

RX(5) OF 16



89%

CON: room temperature

REFERENCE COUNT:

32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 2 OF 10 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 146:337665 CASREACT Full-text

TITLE:

New Pyrrole Inhibitors of Monoamine Oxidase:
 Synthesis, Biological Evaluation, and Structural

Determinants of MAO-A and MAO-B Selectivity

AUTHOR(S): La Regina, Giuseppe; Silvestri, Romano; Artico, Marino; Lavecchia, Antonio; Novellino, Ettore; Befani, Olivia; Turini, Paola; Agostinelli, Enzo

CORPORATE SOURCE: Dipartimento di Studi Farmaceutici, Universita di Roma La Sapienza, Rome, I-00185, Italy

SOURCE: Journal of Medicinal Chemistry (2007), 50(5), 922-931
 CODEN: JMCMAR; ISSN: 0022-2623

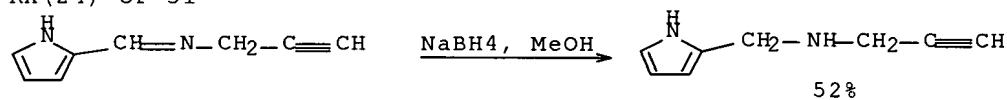
PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal

LANGUAGE:

English

AB A series of new pyrrole derivs. have been synthesized and evaluated for their monoamine oxidase (MAO) A and B inhibitory activity and selectivity. Of these compds., 2-[methyl(benzyl)amino]methyl-1H-pyrrole (I) and 2-(benzylamino)methyl-1-methylpyrrole (II) were the most selective MAO-B (I, SI = 0.0057) and MAO-A (II, SI = 12500) inhibitors, resp. Docking and mol. dynamics simulations gave structural insights into the MAO-A and MAO-B selectivity. Compound II forms an H-bond with Gln215 through its protonated amino group into the MAO-A binding site. This H-bond is absent in the I/MAO-A complex. In contrast, compound I places its Ph ring into an aromatic cage of the MAO-B binding pocket, where it forms charge-transfer interactions. The slightly different binding pose of II into the MAO-B active site seems to be forced by a bulkier Tyr residue, which replaces a smaller Ile residue present in MAO-A.

RX (24) OF 31



CON: STAGE(1) 0 deg C; 45 minutes, room temperature

REFERENCE COUNT:

35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 3 OF 10 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 145:397311 CASREACT Full-text

TITLE: Gold catalysis: phenol synthesis in the presence of functional groups

AUTHOR(S): Hashmi, A. Stephen K.; Weyrauch, Jan P.; Kurpejovic, Elzen; Frost, Tanja M.; Michlich, Burkhard; Frey, Wolfgang; Bats, Jan W.

CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Stuttgart, Stuttgart, 70569, Germany

SOURCE: Chemistry--A European Journal (2006), 12(22), 5806-5814

CODEN: CEUJED; ISSN: 0947-6539

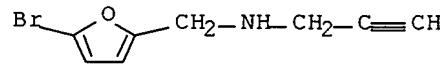
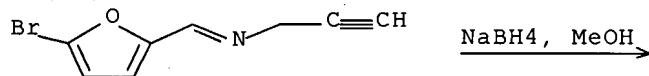
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The effect of different substituents, such as bromo, chloromethyl, hydroxymethyl, formyl, acetyl, carboxy, and acylated hydroxymethyl and ammonium groups, on the furan ring of substrates in gold-catalyzed phenol synthesis has been investigated. The furan ring was also replaced by different heterocycles, such as pyrroles, thiophenes, oxazoles, and a 2,4-dimethoxyphenyl group; gold catalysis then delivered no phenols, but occasionally other products were obtained. [Ru₃(CO)₁₂] also catalyzed the conversion of the furans at a low rate, [Os₃(CO)₁₂] failed as a catalyst, and with [Co₂(CO)₈] the alkyne complex can be obtained, which does not lead to any phenol but reacts with norbornene to give the product of a Pauson-Khand reaction. Efforts to prepare vinylidene complexes of the furans provided the only evidence for these species; in the presence of a phosphine ligand with ruthenium an interesting deoxygenation was observed 5-Methylbenzisofuran-4-methanol was converted to the allyl ether, a building block for para-Claisen rearrangements, and to the aryl triflate, a building block for cross-coupling reactions.

RX (40) OF 88



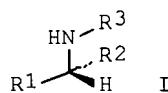
CON: STAGE(1) 10 deg C; 2 hours, room temperature

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 4 OF 10 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 143:78085 CASREACT Full-text
 TITLE: A preparation of amines via asymmetric ruthenium-catalyzed hydrogenation of imines
 INVENTOR(S): Abdur-Rashid, Kamaluddin
 PATENT ASSIGNEE(S): Can.
 SOURCE: PCT Int. Appl., 50 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

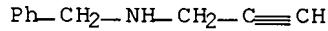
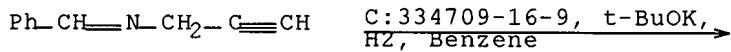
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005056513	A1	20050623	WO 2004-CA2130	20041215
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2549929	A1	20050623	CA 2004-2549929	20041215
PRIORITY APPLN. INFO.:			US 2003-529084P	20031215
			WO 2004-CA2130	20041215

OTHER SOURCE(S): MARPAT 143:78085
 GI



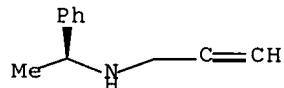
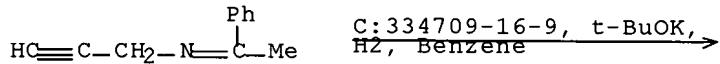
AB The invention relates to a preparation of amines of formula I [wherein: R1 is (hetero)aryl; R2 is H, (hetero)aryl, alkyl, or alk(en/yn)yl, etc.; and R3 is (cyclo)alkyl] via ruthenium-catalyzed hydrogenation of imines of formula R1(R2)C=NR3. The catalytic system includes a ruthenium complex containing (1) a diamine and (2) a diphosphine or two monodentate phosphines ligands. Such process also relates to the asym. hydrogenation of prochiral imines to the chiral amines using chiral ruthenium complexes bearing chiral diphosphines or chiral monodentate phosphines and chiral diamines. For instance, (S)-Ph(Me)CHNH(Me) was prepared via asym. Ru-catalyzed hydrogenation of N-(1-phenylethyldene)methylamine (conversion: 97%, ee: 71%).

RX(10) OF 15



NOTE: 100% conversion, other catalysts gave similar results
CON: 24 hours, room temperature, 15 bar

RX(11) OF 15



NOTE: optimization study (optimized on catalyst), stereoselective
CON: 24 hours, room temperature, 30 bar

REFERENCE COUNT:

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 5 OF 10 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:60158 CASREACT Full-text

TITLE: From D-galactose to enantiopure 3-azabicyclo[3.3.0]octen-7-one derivatives via Pauson-Khand reaction

AUTHOR(S): Areces, Pilar; Carrasco, Esther; Plumet, Joaquin

CORPORATE SOURCE: Facultad de Ciencias, Departamento de Quimica Organica, Universidad de Extremadura, Badajoz, 06071, Spain

SOURCE: ARKIVOC (Gainesville, FL, United States) (2005), (9), 165-174

CODEN: AGFUAR

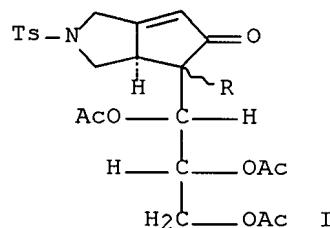
URL: http://www.arkat-usa.org/ark/journal/2005/I09_Molina-Elguero/1293/ME-1293H.pdf

ARKAT USA Inc.

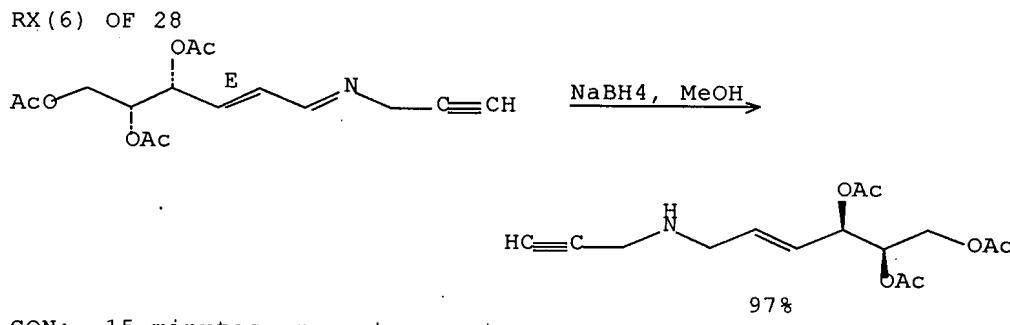
PUBLISHER: Journal; (online computer file)

DOCUMENT TYPE: English

LANGUAGE: GI

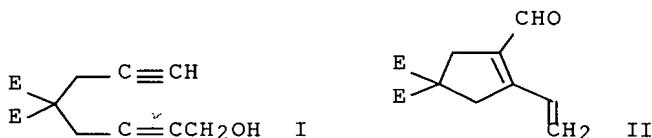


AB The 8-substituted-3-azabicyclo[3.3.0]octen-2-one-7-derivs. I (R = β -, α -H) were obtained in enantiomerically pure form starting from the D-galactose derivative, tri-O-acetyl-D-galactal, in acceptable chemical yield (30%, nine steps) and moderate diastereomeric ratio (18:19 = 2.5:1) via intramol. Pauson-Khand reaction of the appropriate enyne.



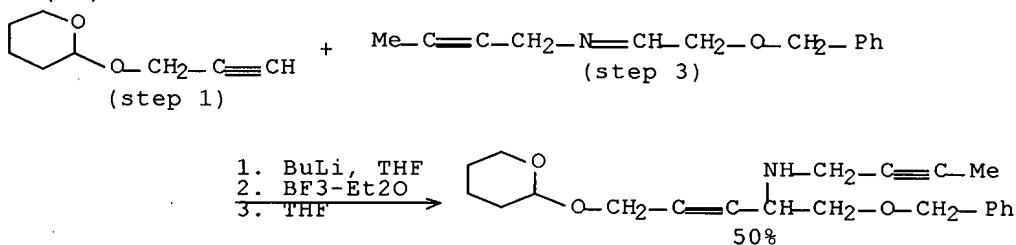
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 6 OF 10 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 142:446756 CASREACT Full-text
 TITLE: Ruthenium-Catalyzed Cycloisomerizations of Diynols
 AUTHOR(S): Trost, Barry M.; Rudd, Michael T.
 CORPORATE SOURCE: Department of Chemistry, Stanford University,
 Stanford, CA, 94305, USA
 SOURCE: Journal of the American Chemical Society (2005),
 127(13), 4763-4776
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB A wide variety of diynols containing tertiary, secondary, and primary propargylic alcs. undergo a cycloisomerization reaction to form dienones and dienals in the presence of a catalytic amount of $[CpRu(CH_3CN)_3]PF_6$. The formation of five- and six-membered rings is possible using this methodol. E.g., $[CpRu(CH_3CN)_3]PF_6$ catalyzed the cycloisomerization of diynol I to give 45% dienal II. Secondary diynols react to form single geometrical isomeric dienones and dienals. Primary diynols undergo a cycloisomerization as well as a hydrative cyclization process. The utility of primary diynol cycloisomerization is demonstrated in a synthesis of (+)- α -kainic acid.

RX(78) OF 534



CON: STAGE {1} 45 minutes, -78 deg C
 STAGE {2} -78 deg C; 10 minutes, -78 deg C
 STAGE {3} -78 deg C; 1 hour, -78 deg C;
 -78 deg C -> room temperature; 1.5 hours, room temperature

REFERENCE COUNT: 106 THERE ARE 106 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 7 OF 10 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 138:73511 CASREACT Full-textTITLE: A novel one-step approach for the preparation of α -amino acids, α -amino amides, and dipeptides from azetidine-2,3-diones

AUTHOR(S): Alcaide, Benito; Almendros, Pedro; Aragoncillo, Cristina

CORPORATE SOURCE: Departamento de Quimica Organica I, Facultad de Quimica, Universidad Complutense de Madrid, Madrid, 28040, Spain

SOURCE: Chemistry--A European Journal (2002), 8(16), 3646-3652
CODEN: CEUJED; ISSN: 0947-6539

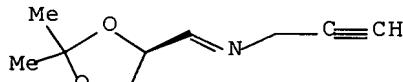
PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

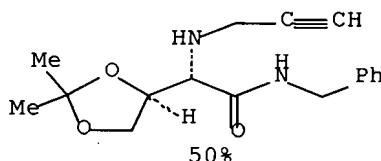
LANGUAGE: English

AB A remarkable reaction of azetidine-2,3-diones with primary as well as secondary amines, and water is presented. Simply by varying the nucleophile, an unprecedented one-step synthesis of α -amino acids, α -amino amides, and dipeptides, was developed in both the racemic and optically pure forms. The current mechanistic hypothesis invokes a concerted process involving CO extrusion. However, a stepwise pathway can also account for these novel transformations.

RX (52) OF 55 - 2 STEPS

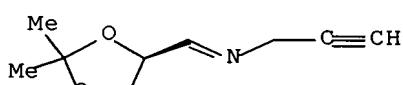


- 1.1. Et₃N,
R:13831-31-7,
CH₂Cl₂
- 1.2. NaOMe, MeOH
- 1.3. (COCl)₂, DMSO,
CH₂Cl₂
- 1.4. Et₃N
2. PhCH₂NH₂, THF

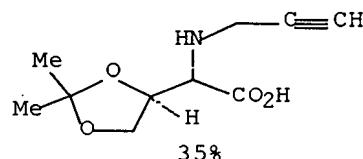


CON: STEP{1.1} room temperature
 STEP{1.2} 0 deg C
 STEP{1.3} 2 hours, -78 deg C
 STEP{2} 2 - 24 hours, room temperature

RX (53) OF 55 - 2 STEPS



- 1.1. Et₃N,
R:13831-31-7,
CH₂Cl₂
- 1.2. NaOMe, MeOH
- 1.3. (COCl)₂, DMSO,
CH₂Cl₂
- 1.4. Et₃N
2. R:13831-31-7,
NH₄Cl, MeOH



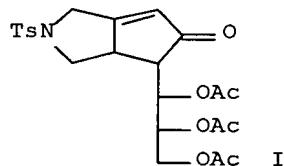
CON: STEP{1.1} room temperature
 STEP{1.2} 0 deg C
 STEP{1.3} 2 hours, -78 deg C
 STEP{2} 2 - 4 days, room temperature

REFERENCE COUNT:

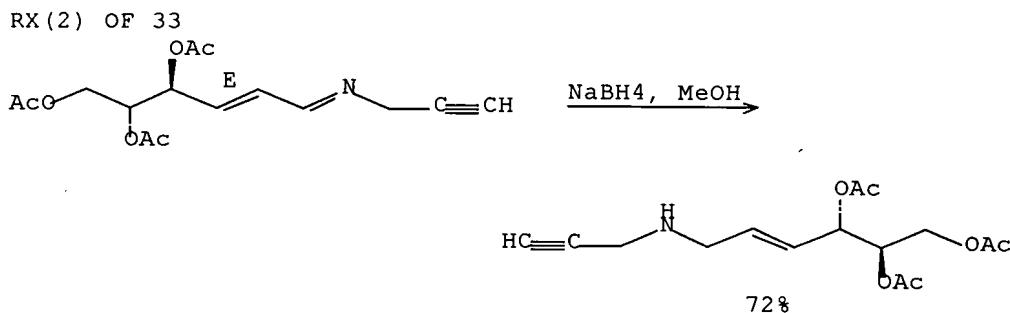
41

THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 8 OF 10 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 137:33178 CASREACT Full-text
 TITLE: Synthesis of Enantiopure 3-Azabicyclo[3.3.0]octen-7-one Derivatives via Intramolecular Pauson-Khand Cycloaddition Reaction Using Tri-O-acetyl-D-glucal as Starting Material
 AUTHOR(S): Areces, Pilar; Duran, M. Angeles; Plumet, Joaquin; Hursthouse, Michael B.; Light, Mark E.
 CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Ciencias, Universidad de Extremadura, Badajoz, 28071, Spain
 SOURCE: Journal of Organic Chemistry (2002), 67(10), 3506-3509
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Some N-substituted 3-azabicyclo[3.3.0]octen-7-one derivs., e.g., I, have been synthesized in an enantiomerically pure form starting from tri-O-acetyl-D-glucal via intramol. Pauson-Khand cycloaddn.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 9 OF 10 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 135:365991 CASREACT Full-text
 TITLE: Mg²⁺-Induced Thermal Enediyne Cyclization at Ambient Temperature

AUTHOR(S):

Rawat, Diwan S.; Zaleski, Jeffrey M.

CORPORATE SOURCE:

Department of Chemistry, Indiana University,
Bloomington, IN, 47405, USA

SOURCE:

Journal of the American Chemical Society (2001),
123(39), 9675-9676

PUBLISHER:

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE:

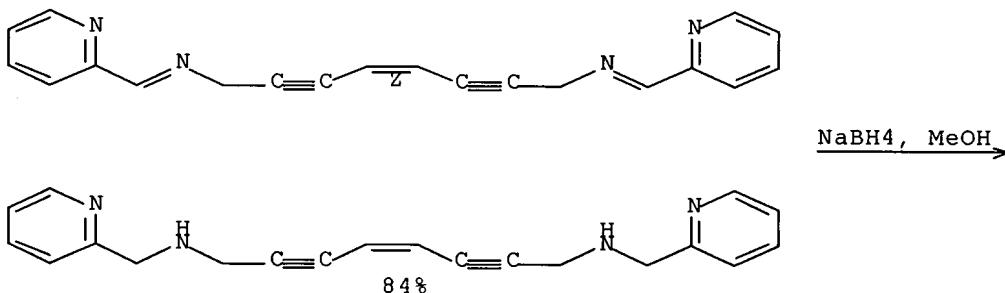
American Chemical Society

LANGUAGE:

Journal

AB Mg²⁺ was used to perform thermal Bergman cyclization thereby demonstrating the use of biol. prevalent and innocuous metals for initiating facile enediyne reactivity. Preparation of Z-[CH(CCCH₂NHCH₂R)₂] (L; R = 2-pyridinyl) and its [MgL]Cl₂ complex as substrates for the cyclization are also reported. Mol. mechanics determined the mol. structure of [MgL]²⁺ using a model including 2 OH⁻ ligands.

RX (2) OF 15



REFERENCE COUNT:

31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 10 OF 10 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 135:210929 CASREACT Full-text

TITLE:

Synthesis of spiro- and fused heterocycles by palladium catalysed carbo- and heteroannulation cascades of allenes

AUTHOR(S):

Grigg, Ronald; Koppen, Ines; Rasparini, Marcello;
Sridharan, Visuvanathar

CORPORATE SOURCE:

Molecular Innovation, Diversity and Automated Synthesis (MIDAS) Centre, School of Chemistry, Leeds University, Leeds, LS2 9JT, UK

SOURCE:

Chemical Communications (Cambridge, United Kingdom) (2001), (11), 964-965

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER:

Royal Society of Chemistry

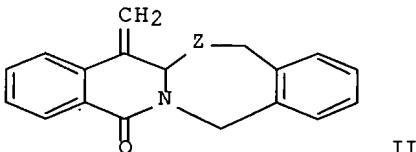
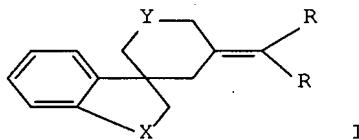
DOCUMENT TYPE:

Journal

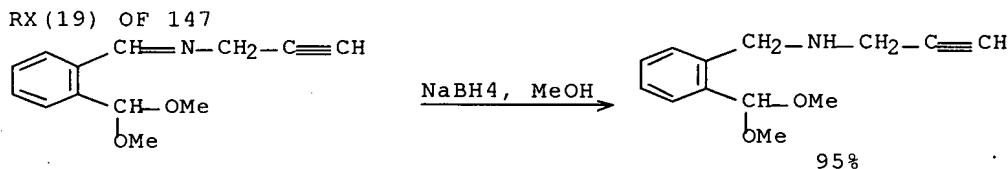
LANGUAGE:

English

GI



AB Two novel palladium catalyzed cascade processes involving the generation of a (π -allyl)palladium intermediate from allenes in an intra- or intermol. fashion, followed by regioselective intramol. nucleophilic addition of amines, alcs. or malonates provide spiro- (I) ($X = NTs, O; Y = N$ -cyclopropyl, NBn, C(CO₂Me)₂; R = H, Me) or linear fused heterocycles (II) (Z = NBn, N-cyclopropyl, N-(1-phenyl)ethyl, N-(1-naphthalen-1-yl)ethyl, O, C(CO₂Me)₂) in good yield.



REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his nofil

(FILE 'HOME' ENTERED AT 11:28:02 ON 20 NOV 2007)

FILE 'BEILSTEIN' ENTERED AT 11:43:24 ON 20 NOV 2007

L1 STR

FILE 'CASREACT' ENTERED AT 11:51:00 ON 20 NOV 2007

L2 8 SEA SSS SAM L1 (99 REACTIONS)

L3 8 SEA ABB=ON PLU=ON L2/COM

FILE 'CAPLUS' ENTERED AT 11:52:35 ON 20 NOV 2007

E US2007-596489/APPS

E WO2004-CA2130/APPS

L4 1 SEA ABB=ON PLU=ON (WO2004-CA2130/AP OR WO2004-CA2130/PRN)
E US2003-529084P/PRN

L5 1 SEA ABB=ON PLU=ON US2003-529084P/PRN

L6 1 SEA ABB=ON PLU=ON L4 OR L5
SEL RN

FILE 'REGISTRY' ENTERED AT 11:53:21 ON 20 NOV 2007

L7 24 SEA ABB=ON PLU=ON (100-46-9/B1 OR 1006-64-0/B1 OR 10137-87-8/
B1 OR 103-67-3/B1 OR 1197-51-9/B1 OR 13280-16-5/B1 OR 14321-27-
8/B1 OR 14683-47-7/B1 OR 19131-99-8/B1 OR 19302-16-0/B1 OR
3466-80-6/B1 OR 441771-18-2/B1 OR 57050-07-4/B1 OR 57734-99-3/B
I OR 618-36-0/B1 OR 622-29-7/B1 OR 626213-92-1/B1 OR 6852-54-6/

BI OR 6907-71-7/BI OR 6907-72-8/BI OR 6907-73-9/BI OR 700-91-4/
 BI OR 855299-36-4/BI OR 855299-37-5/BI)
 D SCA

FILE 'CAPLUS' ENTERED AT 11:54:09 ON 20 NOV 2007
 L8 1 SEA ABB=ON PLU=ON L6 AND L7
 D IALL HITSTR

FILE 'CASREACT' ENTERED AT 11:54:40 ON 20 NOV 2007
 L9 STR
 L10 4 SEA SSS SAM L9 (31 REACTIONS)
 L11 0 SEA SSS SAM L9 AND L1 (0 REACTIONS)

FILE 'STNGUIDE' ENTERED AT 11:57:46 ON 20 NOV 2007

FILE 'CASREACT' ENTERED AT 12:00:58 ON 20 NOV 2007
 L12 QUE ABB=ON PLU=ON (IMINE/FG.RCT OR IMINE/FG.RGT) (L)
 AMINES/FG.PRO
 L*** DEL 8 S L2
 L13 14962 SEA ABB=ON PLU=ON (IMINE/FG.RCT OR IMINE/FG.RGT) (L)
 AMINES/FG.PRO
 L14 50 SEA SUB=L13 SSS SAM L9 (440 REACTIONS)
 L15 43 SEA SUB=L13 SSS SAM L1 AND L9 (170 REACTIONS)
 L16 1057 SEA SUB=L13 SSS FUL L1 AND L9 (3799 REACTIONS)
 L17 1057 SEA ABB=ON PLU=ON L16/COM
 E HYDROGENATION/CT
 L18 7887 SEA ABB=ON PLU=ON HYDROGENATION/CT
 L19 7167 SEA ABB=ON PLU=ON HYDROGENATION CATALYSTS/CT
 L20 91 SEA ABB=ON PLU=ON L17 AND L18
 L21 68 SEA ABB=ON PLU=ON L20 AND L19
 E US2003-529084P/PRN
 L22 1 SEA ABB=ON PLU=ON US2003-529084P/PRN
 L23 1 SEA ABB=ON PLU=ON L22 AND L21
 L24 0 SEA ABB=ON PLU=ON L21 AND ?ASSYM?
 L25 32 SEA ABB=ON PLU=ON L21 AND ?SYMMET?
 L26 39 SEA ABB=ON PLU=ON L21 AND ?ASYM?

FILE 'CASREACT' ENTERED AT 12:06:17 ON 20 NOV 2007

D QUE L26
 D L26 IBIB ABS CRD TOT
 L27 STR
 L28 1 SEA SSS SAM L27 (1 REACTIONS)
 L29 10 SEA SSS FUL L27 (12 REACTIONS)
 L30 10 SEA ABB=ON PLU=ON L29/COM
 D QUE L30
 D L30 IBIB ABS CRD TOT